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Interaction Energies and Electronic Spectra of Fluorene-Receptors Molecules for Carbon Dioxide Detection

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By

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Interaction energies and electronic spectra of fluorene-receptors molecules for carbon dioxide detection

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The world's oceans absorb a significant percentage of anthropogenic carbon emissions, and CO_2 levels have profound effects on the marine environment. Of primary concern is the acidification of the oceans due to dissolved CO_2. The goal of this research is to design new sensing technologies for deployment in the marine environment to detect CO_2 pollutant. A series of carbon dioxide (CO_2) receptors that are complexed to fluorene oligomers were studied computationally.

In chapter 1, an overview of CO_2 chemistry and various CO_2 sensors is discussed. A short overview of the method (Kohn-Sham density functional theory and time-dependent density functional theory (TDDFT)) employed in this work is given.

Chapter 2 presents a study on the interaction energy and electronic excitations of fluorene-receptors as CO_2 sensors. From our results, the monomer-receptor complexes show remarkable redshifts in their absorption spectra, which decrease on moving to dimer and trimer-receptor complexes (all blue-shifted).

DEDICATION

I would like to dedicate this thesis to

Bezaleel ElShalom

ACKNOWLEDGEMENTS

"Now thanks *be* to God who always leads us in triumph in Christ Jesus."

II Corinthians 2:14

To begin with, I would like to express my deepest appreciation to the Lord Almighty, the creator of the universe for His protection, guidance, and grace through my graduate studies and research. To my wife, I cannot thank you enough for all that you do but say, "*Je t'aime beaucoup!"* I want to thank my parents and siblings for their continuous support, encouragement, and sacrifices.

I would like to express my sincere appreciation to my research advisor, Dr. Steven R. Gwaltney for his patience, guidance and constructive critique of this research. Thank you for providing me the opportunity to carry out research under your direction even while I was a novice. And thanks to your family as well. Also, to my graduate committee members, Dr. Scott Colleen, and Dr. Todd Mlsna, I would like to say thank you for your advice and support. Thank you to the Department of Chemistry, Mississippi State University, and Mississippi EPSCoR for providing financial assistance throughout the program.

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Dotse, Prakash Khanal, my office mates, and all my friends in WEMMI Starkville fellowship and Starkville Church of God.

À Dieu soit la gloire !

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CHAPTER I

INTRODUCTION

1.1 Carbon dioxide chemistry

Carbon dioxide is a colorless gas made up of a carbon atom covalently bonded (double bond) to two oxygen atoms; the carbon-oxygen bonds are equivalent and are noticeably shorter (1.16 Å) than a typical C-O single bond (1.43 Å).[1] CO_2 is a natural greenhouse gas present in the earth's atmosphere.[2] It constantly circulates in the environment through various processes known as the carbon cycle. Industrial processes, volcanoes, and human activities such as burning of wood and fossil fuels release large amounts of CO_2 into the air. Even though CO_2 absorption and release are always occurring because of natural processes, there is a global concern due to increased CO_2 concentration and its serious impact on the environment. Its concentration has risen by 30% since the nineteenth century and may double or triple in the next century.[2,3] A significant percentage of anthropogenic carbon emissions is absorbed by the oceans, lakes, and rivers, creating a major negative impact on the marine ecosystem over time due to ocean acidification.[4,5]

Carbon dioxide is generally perceived as a highly inert gas with a low reactivity due to its high chemical stability.[6] Also, CO_2 has no permanent dipole moment due to its centrosymmetric nature. However, its large quadrupole moment due to the charge separation in the C=O bonds leads to quadrupole-dipole interactions and quadrupole-

induced dipole interactions.[7] The reactivity of CO_2 with other molecules can occur via three modes: through the nucleophilic oxygen atom, the electrophilic carbon atom, and its pi system.[6,8,9]

1.2 Brief Overview of CO_2 sensors

The term sensor is defined as "a receptor that interacts with an analyte to produce a detectable change in signal."[10] These signals can be current, absorbance, mass, or acoustic waves.[11] Detection of the analyte can be direct, for which a change in signal is observed when the analyte binds to a receptor, or via an indicator displacement assay in which an analyte displaces an indicator bound to the receptor.[10,12] Several methods have been developed for CO_2 measurement and are broadly classified as optical and electrochemical sensors. This short overview will focus on Severinghaus electrode sensors, optical sensors, metal-oxide sensors, and polymer-based sensors.

1.2.1 Severinghaus CO_2 sensors

Several sensors for CO_2 measurement have been presented in the literature. One of the oldest is based on the Severinghaus electrode. It was developed in 1958 by John W. Severinghaus and A. Freeman Bradley. The sensor consists of a glass electrode filled with aqueous bicarbonate solution and is covered with a selective membrane permeable to CO_2 but impermeable to ions.[13,14] When CO_2 diffuses into the solution, there is a resulting change in the pH of the electrolyte solution, which is measured with a pH probe.

Some disadvantages of this sensor are the high cost of maintenance, interference of other gases, and indirect measurement of CO_2 (CO_2 is measured in the ionic form).

1.2.2 Optical sensors

Optical sensors for detection of an analyte are based on the absorption or emission of light. These sensors can monitor analytes in the infrared region or the ultraviolet-visible region of the electromagnetic spectrum. Optical sensors possess various merits such as high sensitivity, ease of usage, wide dynamic range, and low cost compared to the conventional sensors.

The most common optical method for CO_2 detection is based on infrared absorption due to CO_2's strong absorption in this region.[14,15,16] However, there is a major drawback due to interference of carbon monoxide and water vapor, as well as the bulkiness of some of these detectors.[14]

Other optical methods, such as colorimetric, luminescent, and fluorescent, have been applied to the detection of CO_2.[16,17,18]

1.2.3 Metal oxide sensors

Metal oxide sensors have currently gained much attention, and a lot of research has been invested in gas sensing. This is due to their low cost, robustness, long-term stability, and ease of use.[14,19] They are made up of a sensitive layer deposited over a substrate with electrodes. The interaction of the gas with the metal oxide can be achieved by measuring the change in work function, conductivity, or capacitance.[19] Upon

interaction of CO_2 gas with a metal oxide, the gas dissociates into ions or forms complexes, resulting in the transfer of electrons, which causes a change in the resistance of the surface layer. This change is directly related to the CO_2 concentration present. Metal oxides for gas sensing are categorized into two groups: transition-metal oxides such as Cr_2O_3, CuO, and TiO and non-transition metal oxides such as SnO_2, and In_2O_3. Several papers have been published on metal oxide gas sensors, and the major focus is the enhancement of their sensitivity.[19]

1.2.4 Polymer-based sensors

Conducting polymers (CP) have gained much attention over the past decades for their use as biological and chemical sensors. This is due to their ease of synthesis, high sensitivities, and short response time and the ability to fine-tune their chemical and physical properties for specific needs.[11,20] A number of papers[21,22,23] and literature reviews[11,24,25] on the use of conducting polymers for various kinds of gas detection have been published. Due to the intrinsic properties of conducting polymers, reacting with an analyte or gas results in a change in their electrical conductivity. The most widely explored conducting polymers for gas sensing are polyaniline, polypyrrole, and polythiophene.[11,24]

Those polymer-based sensors used for CO_2 detection have amino groups in them. Several studies have shown that the interaction between the amino group and CO_2 is an acid-base reaction. The electron-deficient C atom of CO_2 acts a hard acid, which can interact with the N atom, that acts as a hard base.[2,26,27,28]

1.3 Kohn-Sham density functional theory (KS-DFT)

Density functional theory (DFT) is an alternative to wave function theory in which the many-electron problem is formulated in terms of the electron density to generate the energy of a molecule.

The Hamiltonian for an interacting system is

$$\hat{\mathrm{H}} = T + V + W \,, \tag{1.1}$$

where T is the electronic kinetic energy operator

$$T = \sum_i^N \frac{-\nabla^2}{2} \,, \tag{1.2}$$

V is the energy due to the nuclear-electron attraction

$$V = \sum_{\mathrm{i}}^{\mathrm{N}} \upsilon\,(\mathrm{r_i}) \;\; , \tag{1.3}$$

and W is the electron-electron interacting energy.

Solutions to the Schrödinger equation

$$\hat{\mathrm{H}}\Psi = \mathrm{E}\Psi \;\; , \tag{1.4}$$

are wave functions $\Psi(\mathrm{x_1 x_2} \ldots \mathrm{x_N})$, where $\mathrm{x_i}$ is the product of the spin and space coordinates.

E is the total energy of the interacting system, which is given by

$$\mathrm{E}[\rho] = \mathrm{T}[\rho] + \int \upsilon(\mathrm{r})\rho(\mathrm{r})\mathrm{dr} + \mathrm{W}[\rho] \,, \tag{1.5}$$

where ρ is the electron density

$$\rho(r_1) = N \int \ldots \int |\Psi(\mathrm{x_1 x_2} \ldots \mathrm{x_N})|^2 ds_1 dx_2 \ldots \mathrm{dx}_N \tag{1.6}$$

In the Kohn-Sham approach,[29] a fictious system of non-interacting electrons is constructed in such a way that the density generated is the same as that of the interacting system. For the non-interacting system, the energy (eqn. 1.5) was reformulated as

$$E[\rho] = T_s[\rho] + \int \upsilon(r)\rho(r)dr + W[\rho] + J[\rho] + E_{xc}[\rho]\,, \tag{1.7}$$

where T_s is the kinetic energy for the non-interacting system,

J[ρ] is the classical Coulomb energy

$$J[\rho] = \frac{1}{2}\iint \frac{\rho(r)\rho(r')}{|r-r'|}\, drdr'\,, \tag{1.8}$$

and E_{xc} is the exchange-correlation functional

$$E_{xc}[\rho] = (T[\rho] - T_s[\rho]) + \{\upsilon(r)\rho(r) - J[\rho]\}\,. \tag{1.9}$$

The Kohn-Sham equations are determined by solving the total energy variationally, which yields the Kohn-Sham potential, υ_s

$$\upsilon_s = \upsilon_0(r) + \int \frac{\rho(r')}{|r-r'|}\, dr' + \upsilon_{xc}(r), \tag{1.10}$$

where υ_{xc} is the exchange-correlation potential

$$\upsilon_s = \frac{\delta E_{xc}[\rho]}{\delta\rho(r)}\,. \tag{1.11}$$

Since the Kohn-Sham method is applied to a non-interacting system, the wavefunction is a single Slater determinant constructed from a set of orbitals which are the solutions to the one-particle Schrödinger equation

$$\left(\frac{-\nabla^2}{2} + \upsilon_s\right)\phi_i(r) = \epsilon_i\phi_i(r)\,. \tag{1.12}$$

The density is determined by setting

$$\rho(r) = \sum_i^N |\phi_i|^2\,, \tag{1.13}$$

where N is the number of electrons.

The Kohn-Sham equations are then solved self-consistently: one begins with a guess at $\rho(r)$ to generate υ_s from eqns. 1.10 and 1.11 then solves eqn. 1.12 to generate a new $\rho(r)$ from ϕ_i.

1.4 Time-dependent density functional theory (TDDFT)

Time-dependent density functional theory (TDDFT) has become one of the most successful and most widely-used tools for calculating excited state properties of medium to large molecular systems.[30,31] The TDDFT formalism is based on the Runge-Gross theorem,[32] which is an extension of the first Hohenberg-Kohn theorem to time-dependent systems.

The Runge-Gross theorem is derived for a system of N electrons moving in an external time-dependent electric field υ (r, t). The N-electron wavefunction satisfies the time-dependent Schrodinger equation:

$$\hat{\mathrm{H}}(r,t)\left|\Psi(r,t)\right\rangle = i\frac{\partial}{\partial t}|\Psi(r,t)\rangle, \tag{1.14}$$

where the total Hamiltonian, H takes the form

$$\hat{\mathrm{H}}(r,t) = \mathrm{T} + V_{ext} + W, \tag{1.15}$$

and T is the sum of the kinetic energies, W is the electron-electron interaction, and V is the external potential. The external potential determines the wavefunction and the electron density. The total electron density is given in eqn. 1.6. The Runge-Gross theorem shows that there is a one-to-one mapping between the time-dependent electron density and the time-dependent external potential of the system.

The KS equation in the time-dependent form is

$$i\frac{\partial}{\partial t}\phi_i(r,t) = [\frac{-\nabla^2}{2} + \upsilon(r,t) + \int \frac{\rho(r,t)}{r_{12}}dr + \upsilon_{xc}(r,t)]\phi_i(r,t) \qquad (1.16)$$

where ϕ_i are the single electron orbitals used to construct the density, ρ(r, t) (eqn. 1.13).

The excitation energies in TDDFT are obtained through linear response theory.[31] Linear response TDDFT is mostly used for calculations of electronic absorption spectra of molecules. In this theory, an N-electron system, originally in its ground stationary state, is exposed to a time-dependent perturbation, $\upsilon_{appl}(\omega)$. The dynamic equation to the perturbation is

$$\left\{\omega\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} - \begin{bmatrix}A & B\\ B^* & A^*\end{bmatrix}\right\}\begin{pmatrix}\delta p(\omega)\\ \delta p(\omega)\end{pmatrix} = \begin{pmatrix}\upsilon_{appl}(\omega)\\ \upsilon_{appl}(\omega)\end{pmatrix}, \qquad (1.17)$$

where A and B are the Hessians of the electronic energy. The two-electron integrals A and B (in Mulliken notation) are given as

$$\mathrm{A_{ia,jb}} = \delta_{\mathrm{i,j}}\ \delta_{\mathrm{a,b}}(\epsilon_{\mathrm{a}} - \epsilon_{\mathrm{i}}) + (\mathrm{ia|jb}) + (\mathrm{ia|f_{xc}|jb}) \qquad (1.18)$$

$$\mathrm{B_{ia,jb}} = (\mathrm{ia|bj}) + (\mathrm{ia|f_{xc}|bj}) \qquad (1.19)$$

$$\mathrm{f_{xc}} = \frac{\delta \mathrm{V_{xc}[\rho]}}{\delta \rho(\mathrm{r})} \qquad (1.20)$$

where f_{xc} is the exchange kernel, ϵ are KS orbital energies, and a, b, i, j are KS orbitals.

The excitation energies and oscillator strengths are extracted by rearranging equation 1.17 to take the form of a dynamic polarizability α(ω) using the sum-over-states theorem

$$\alpha(\omega) = \sum_{I\neq o}\frac{f_I}{\omega_I^2 - \omega^2}, \qquad (1.21)$$

where $$f_I = \frac{2}{3}\omega_I \sum_{q=x,y,z}|\langle\Psi_0|q|\Psi_I\rangle| \qquad (1.22)$$

is the oscillator strength. Ψ_o and Ψ_I refer to the ground and excited stationary states respectively. The associated excitation energy obtained is

$$\omega_I = E_I - E_0 \tag{1.23}$$

Equation 1.17 can be reduced to a matrix pseudo-eigenvalue problem,

$$\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{pmatrix} X_I \\ Y_I \end{pmatrix} = \omega_I \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{bmatrix} \begin{pmatrix} X_I \\ Y_I \end{pmatrix} \tag{1.24}$$

which contains paired excitation ($\omega_I > 0$) and de-excitation ($\omega_I < 0$) solutions.

Neglecting the B matrices in Eq. 1.25 results in a Hermitian eigenvalue equation,

$$\mathbf{A}\mathrm{X_I} = \boldsymbol{\omega}_\mathrm{I} X_\mathrm{I} \,. \tag{1.25}$$

This is called the DFT Tamm-Dancoff approximation (TDA) by Hirata and Head-Gordon.[33]

CHAPTER II

INTERACTION ENERGIES AND ELECTRONIC SPECTRA OF FLUORENE-RECEPTOR MOLECULES FOR CARBON DIOXIDE DETECTION

2.1 Abstract

We report a study on a series of carbon dioxide (CO_2) receptors that are complexed to fluorene oligomers. The structural, electronic, and optical properties of these receptor complexes have been determined computationally. The interactions of the receptors and the fluorene-receptor complexes with CO_2 are investigated using resolution-of-identity Møller-Plesset second-order perturbation theory (RI-MP2) and density functional theory with dispersion correction (ωB97X-D3) with the aug-cc-pVTZ basis. Lewis acid-Lewis base interactions between the carbon of CO_2 and a nitrogen of the receptor molecules, along with weak hydrogen bonds, stabilize the complexes. Qualitative results of the binding energy of CO_2 with the receptors and the fluorene-receptor complexes are reported. In addition, time-dependent density functional theory is employed to describe the electronic properties of the CO_2 complexes. The monomer-receptor complexes show remarkable redshifts in their absorption spectra, which decrease on moving to dimer and trimer-receptor complexes (all blue-shifted). This effect is much stronger in water than in the gas phase. Finally, natural bond orbital (NBO) charge analysis and electron

attachment/detachment density plots are presented to analyze the nature of the electronic excitations.

2.2 Introduction

Carbon dioxide is a greenhouse gas naturally present in the earth's atmosphere.[2] As a product of fossil fuel combustion, its increasing concentration and serious impact on the environment have been major concerns for those seeking greenhouse reduction.[34,35,36] The world's oceans absorb a significant percentage of anthropogenic carbon emissions, with CO_2 levels having a profound effect on the marine ecosystem. Of primary concern is the acidification of the oceans due to dissolved CO_2.[5] This acidification results in a decline in the pH level, resulting in negative impacts on marine life. This condition has necessitated the development of robust sensors for water quality monitoring due to poor sensitivity and stability of current shipboard sensors.[37] Hence, the development of CO_2 sensors remains an active area of research.

Several CO_2 sensors have been designed over the years which differ based on different sensing mechanisms. The conventional systems for CO_2 detection are the Severinghaus-type sensors,[13,14] non-destructive infrared (NDIR),[14] gas chromatography (GC), and mass spectrometers (MS).[38,39] In the last decades, the potential offered by polymer-based sensors has been realized to a large extent due to their inherent properties.[11,20,40] Conducting polymers (CP's) over the years have shown great potential for their use as biological and chemical sensors due to their ease of synthesis, their electrical conductivity, and the ability to fine-tune their chemical and physical properties for specific needs. Various schemes such as conductometric, potentiometric, colorimetric, and fluorescent detection have been developed to design CP-based sensors.[20] Among

these, the fluorescence-based methods have expanded rapidly and have gained wider applications due to their high sensitivity, versatility, noninvasiveness, and low toxicity.[41] CP's may also be modified by incorporating receptors to enhance their affinity for analytes.

CO_2 is a stable molecule with no permanent dipole moment. However, the large quadrupole moment of CO_2, due to the charge separation in the C=O bonds, leads to quadrupole-dipole interactions and quadrupole-induced dipole interactions,[7] thus enabling CO_2 to act as a Lewis acid and a Lewis base. Ab initio calculations[7,9,28,42] and spectroscopic evidence[2,27,43] have shown that in the presence of Lewis bases such as amines, alcohols, and esters, the carbon atom of CO_2 interacts with the electron-rich sites of these compounds to form electron donor-acceptor (EDA) complexes. In this study, theoretical calculations were carried out to delineate the interaction of the receptor and fluorene-receptor molecules with CO_2 and to determine the absorption spectra of the complexes.

2.3 Computational details

Geometries of receptors and receptor-CO_2 complexes were fully optimized using the was resolution of the identity (RI) approximation to the second-order Møller-Plesset (MP2)[44] perturbation theory with the cc-pVTZ basis set.[45] For the parent *n* fluorene, where *n* is the number of repeating unit and *n* fluorene- CO_2 complexes, the ωB97X-D3[46] functional with the def2-TZVP basis set[47] was employed due to convergence problems using the RI-MP2 method. The geometries were fully optimized without symmetry constraints. Single point (SP) calculations using ωB97X-D3/aug-cc-pVTZ (and RI-MP2 for only the receptor complexes) were performed on the optimized geometries of the receptor-CO_2

and fluorene-receptor-CO_2 complexes. Since the interaction in our system is relatively weak, basis set superposition error (BSSE) can be a major contribution to the interaction energy. Therefore, the interaction energies (ΔE) between receptors and CO_2 were calculated with BSSE correction by applying the counterpoise (CP) correction.[48] The interaction energy (ΔE) and counterpoise corrected energy (ΔE_{cp}) are defined in Eqs. (2.15) and (2.16), respectively.

$$\Delta E = E_{complex} - E_{receptor} - E_{analyte} \quad (2.15)$$

$$\Delta E_{CP} = \Delta E - \Delta E_{BSSE} \quad (2.16)$$

To describe the electronic properties of the complexes, vertical singlet-singlet excitation energies and oscillator strengths were elucidated by TDDFT. TD-ωB97X-D/def2-SVPD was employed for all calculations in the gas and aqueous phases. Natural bond orbital (NBO) calculations were performed using the NBO package[49] to describe any migration of electron density in the complexes with ωB97X-D/def2-SVPD. Electron attachment/detachment density analyses[50,51] were also carried out to help understand the nature of electronic excitations with the same functional and basis set. All calculations were performed with a developer's version of Q-Chem 5.[52] Molecular structures were visualized with the visual molecular dynamics (VMD) program.[53] To capture solvent effects, the polarizable continuum model (PCM)[54,55] as implemented in Q-Chem[52] was used.

2.4 Results and Discussion

2.4.1 Structural properties

The optimized structures of receptor-CO_2 complexes and fluorene-receptor-CO_2

complexes are displayed in Fig. 2.1 – 2.7. Structural parameters of complexes such as adsorption distance (d_{N--C}), and OCO bond angle (<OCO) are summarized in Table 2.1.

The gas phase calculations on the receptor-complexes give the adsorption distances (d_{N--C}) as 2.79, 2.99, and 3.06 Å, while the OCO bond angles are 176.32, 177.10, and 177.79 degrees for A1-CO_2, A2-CO_2, and A3-CO_2 respectively. The adsorption distances and OCO angles for A1-CO_2, A2-CO_2, and A3-CO_2 in the gas phase were almost the same as in the aqueous phase (see Table 2.1). From our calculations, we observe that adsorption distance (d_{N--C}) and OCO bond angle (<OCO) for the receptors and for the fluorene-receptor molecules are almost the same in the gas phase but vary in the aqueous phase. In the case of fluorene-receptor complexes, specifically the monomer and dimer, the structural parameters were substantially different in the aqueous phase. According to Table 2.1, the $d_{N—C}$ bond distance decreased by about 1.3 Å in the aqueous phase, from the receptor complexes to both the monomer and dimer complexes, but the distance increased in the trimer complexes. The deformation of the OCO bond angle and deviation of O-C bond length is an indication of an increase in the interaction of fluorene-receptor molecules with the analyte. For the monomer and dimer (in the aqueous phase), the OCO deformation angle from linearity (180˚) increases substantially when compared to the trimer and receptor complexes (Fig 2.1 - 2.7 and Table 2.1). This is an indication that the interaction between fluorene-receptors with the analyte decreases at the longest chain length.

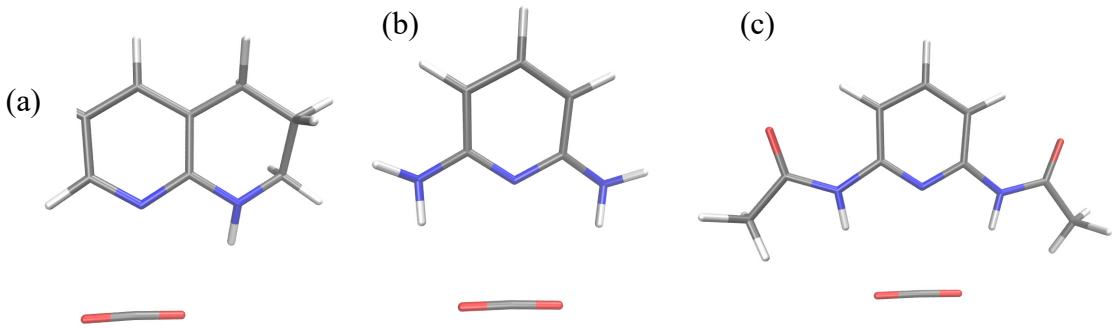


Figure 2.1 RI-MP2/cc-pVTZ optimized structures of receptor-CO_2 complexes in the aqueous phase (a) A1-CO_2 (b) A2-CO_2 (c) A3-CO_2

Color code: N - blue, C - silver, O - red, H- white.

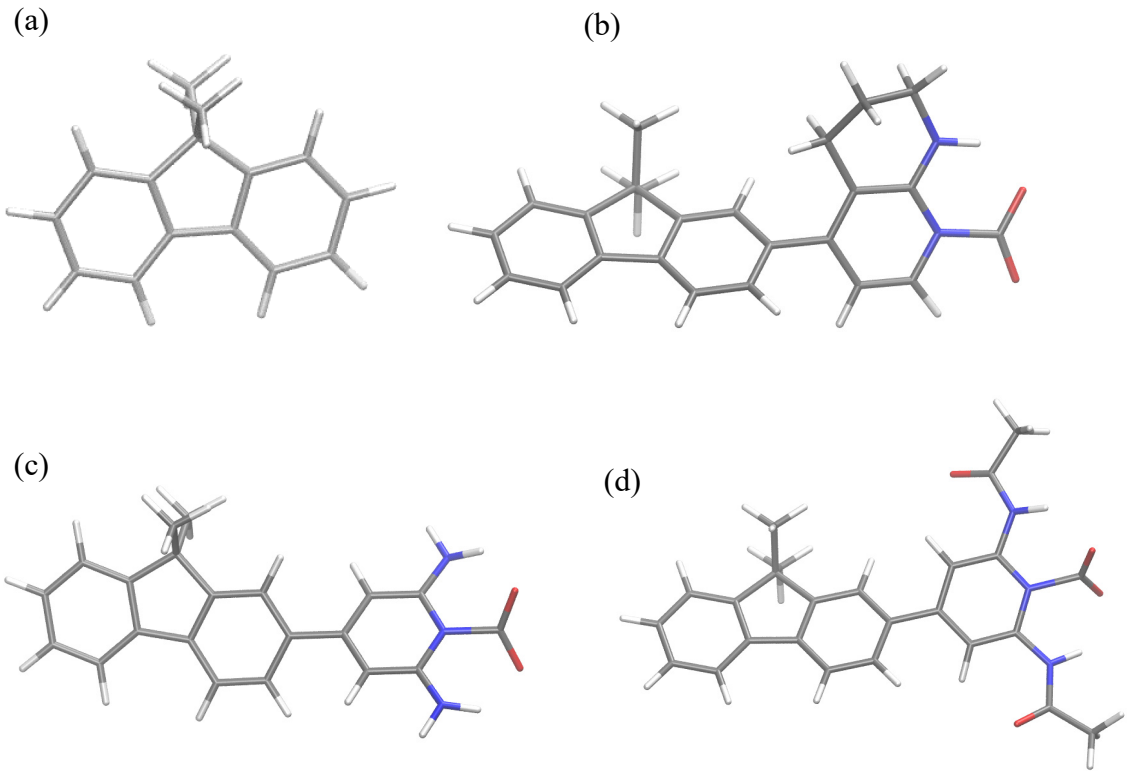


Figure 2.2 ωB97X-D3/def2-TZVP optimized structures of the fluorene monomer (a), and fluorene-receptor-CO_2 complexes in aqueous phase: (b) MA1-CO_2 (c) MA2-CO_2 (d) MA3-CO_2

Color code: N - blue, C - silver, O - red, H- white.

(a)

(b)

(c)

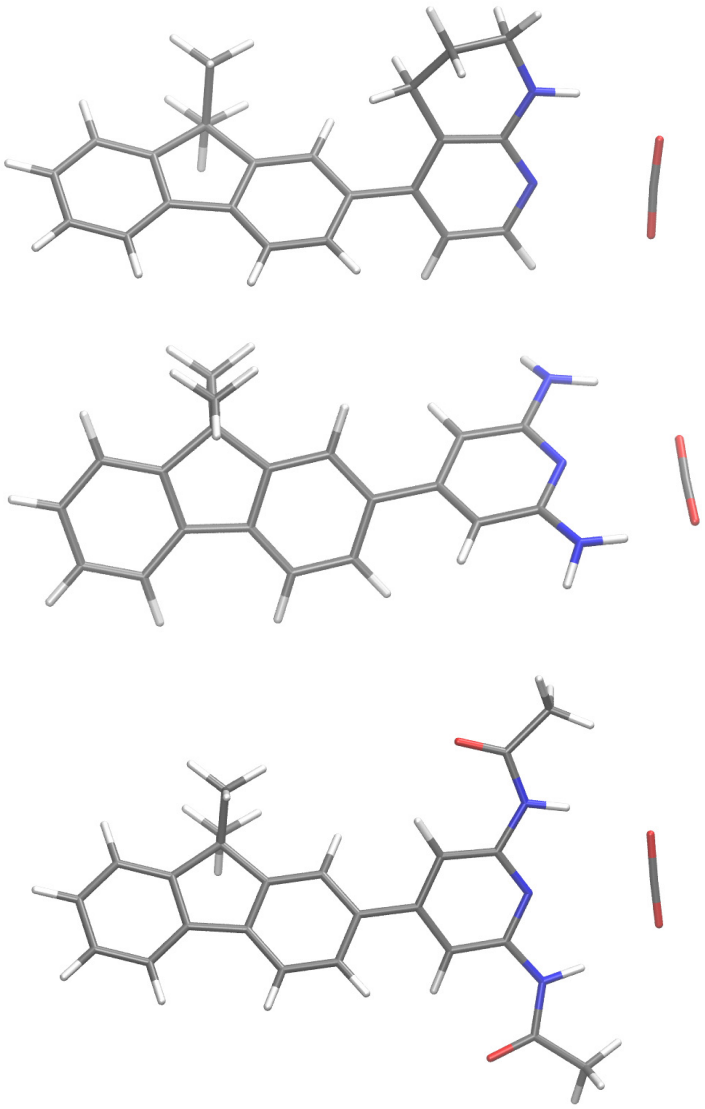


Figure 2.3 ωB97X-D3/def2-TZVP optimized structures of monomer-receptor-CO_2 complexes in the gas phase. (a) MA1-CO_2 (b) MA2-CO_2 (c) MA3-CO_2

Color code: N - blue, C - silver, O - red, H- white.

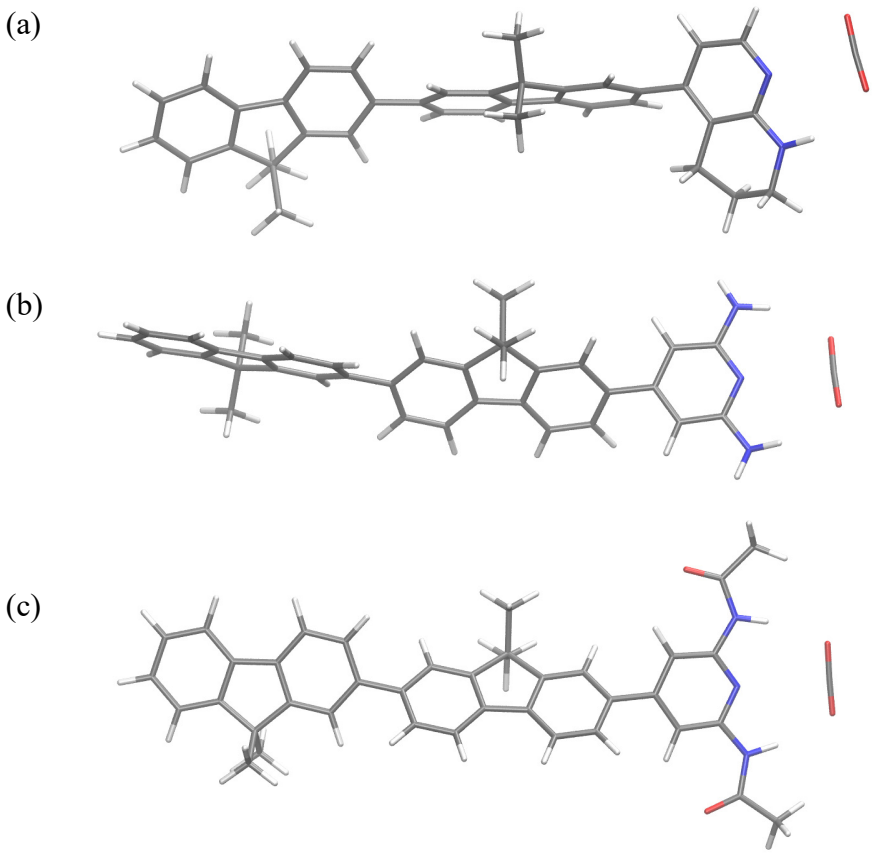
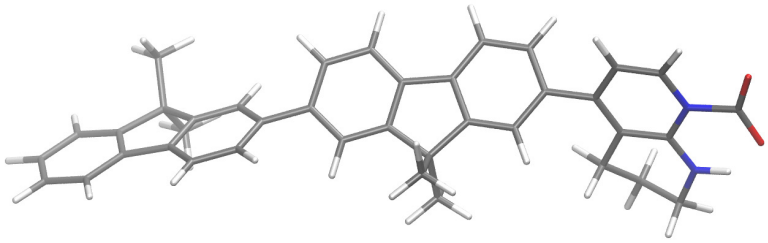
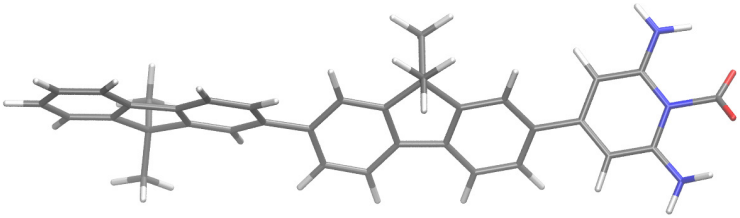


Figure 2.4 ωB97X-D3/def2-TZVP optimized structures of dimer-receptor-CO_2 complexes in the gas phase. (a) DA1-CO_2 (b) DA2-CO_2 (c) DA3-CO_2

(a)



(b)



(c)

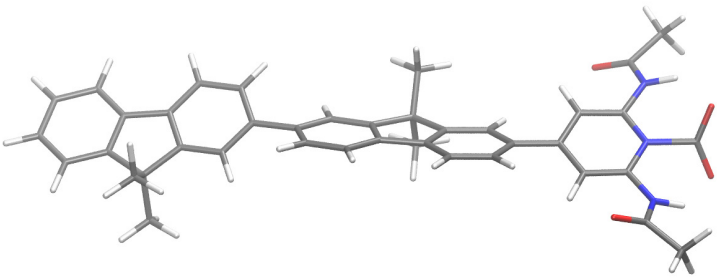


Figure 2.5 ωB97X-D3/def2-TZVP optimized structures of dimer-receptor-CO_2 complexes in the aqueous phase. (a) DA1-CO_2 (b) DA2-CO_2 (c) DA3-CO_2

(a)

(b)

(c)

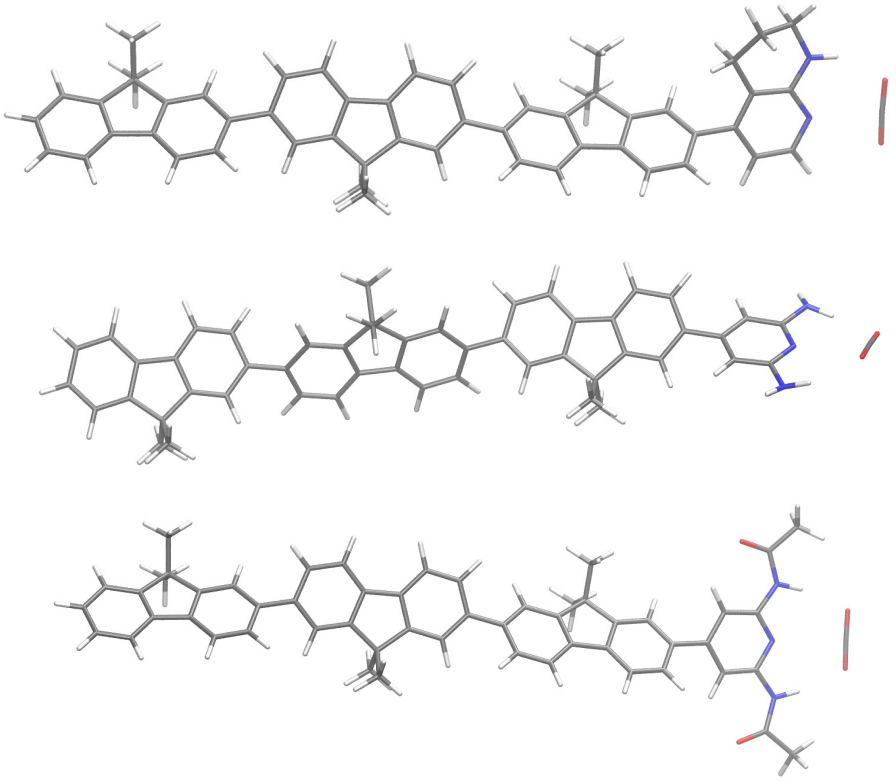
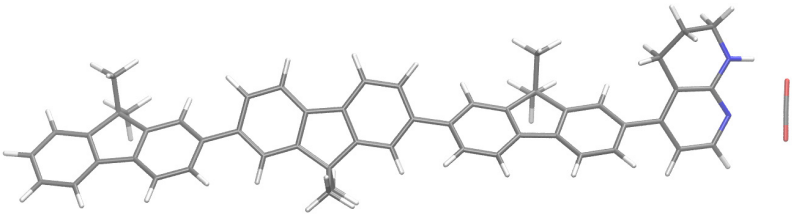
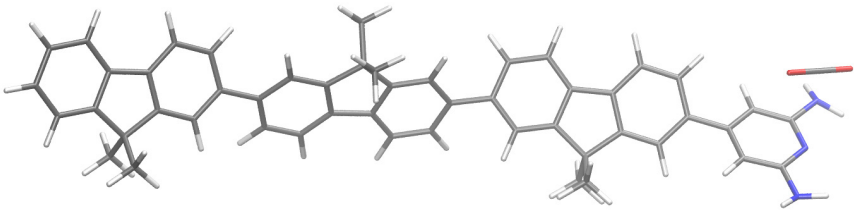


Figure 2.6 ωB97X-D3/def2-TZVP optimized structures of trimer-receptor-CO_2 complexes in the gas phase. (a) TA1-CO_2 (b) TA2-CO_2 (c) TA3-CO_2

(a)



(b)



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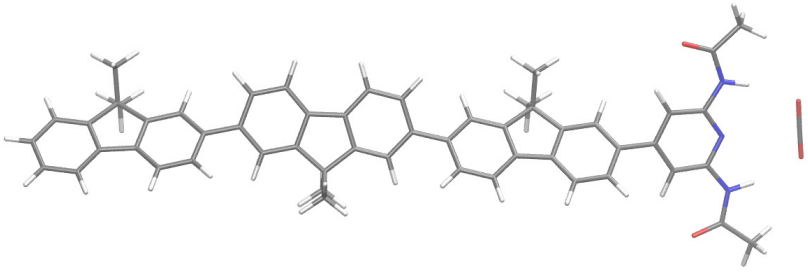

Figure 2.7 ωB97X-D3/def2-TZVP optimized structures of trimer-receptor-CO_2 complexes in water. (a) TA1-CO_2 (b) TA2-CO_2 (c) TA3-CO_2

Table 2.1 ωB97X-D3/aug-cc-pVTZ distances between the carbon of CO_2 and the respective nitrogen of the aromatic systems d(N-C) [Å], O-C-O angle, and calculated interaction energy (ΔE). Values of bond distance d(N-C) and OCO angles in parentheses are the aqueous phase values. RI-MP2/aug-cc-pVTZ interaction energies for receptors only are denoted in italics

Complexes	d(N-C) (Å)	<OCO (°)	ΔE (kcal/mol)
Receptor-complexes			
A1-CO2	2.79 (2.76)	176.32 (175.53)	-5.46 *(5.41)*
A2-CO2	2.99 (2.95)	177.10 (177.04)	-5.22 *(-5.27)*
A3-CO2	3.06 (3.05)	177.79 (179.20)	-5.76 *(-5.75)*
Monomer-receptor-complexes			
MA1-CO2	2.80 (1.54)	175.81 (131.28)	-5.62
MA2-CO2	2.99 (1.55)	176.92 (133.03)	-5.23
MA3-CO2	3.11 (1.59)	177.87 (135.35)	-5.70
Dimer-receptor-complexes			
DA1-CO2	2.81 (1.54)	175.90 (131.35)	-5.54
DA2-CO2	2.97 (1.55)	176.80 (132.97)	-5.46
DA3-CO2	3.08 (1.59)	177.75 (135.31)	-5.75
Trimer-receptor-complexes			
TA1-CO2	2.80 (2.97)	175.86 (177.70)	-5.61
TA2-CO2	2.97 (3.40)	176.79 (179.47)	-5.42
TA3-CO2	3.10 (3.18)	177.86 (178.92)	-5.75

2.4.2 Understanding CO_2 interactions with receptors

To examine the reactivity of the receptors to CO_2, the interaction energies of the complexes were evaluated with ωB97X-D3/aug-cc-pVTZ on the various optimized structures. Since these complexes are stabilized to a large extent by van der Waals interactions, the range-separated hybrid functional with the Grimme D3 empirical dispersion correction (ωB97X-D3) was chosen due to the failure of conventional DFT functionals to describe dispersion effects.[56] The BSSE correction was also taken into account for all the interaction energies for the complexes in the gas phase. The interactions between the receptors and CO_2 are mainly electrostatic and are between the carbon of the CO_2 and the nitrogen of the receptor. This contribution arises from the electron-deficient carbon atom of CO_2 acting as a Lewis acid with the nitrogen atom of the receptors acting as a Lewis base. Also, there is a weak hydrogen bond contribution to the stabilization of these complexes between the proximal hydrogen atoms of the receptors and the oxygen atoms of CO_2.

We report our calculated interaction energies (in kcal/mol) of these complexes in the gas phase. From the structural parameters (Table 2.1), we observe that the adsorption distance and OCO deformation angle is greater in A1 than in the other two receptors (A2 and A3), which suggests that A1 could have a greater stabilization energy. However, that was not observed in our calculations (Table 2.1). A3 forms the most stable complex with CO_2, with a binding energy of -5.76 kcal/mol, calculated with ωB97X-D3/aug-cc-pVTZ in the gas phase. The stronger binding of A3 with CO_2 can be attributed to the extra hydrogen bond between the proximal hydrogen atoms and the oxygen atoms of CO_2. However, A2 exhibits an extra hydrogen bond as does A3; thus, it can be deduced that the

electron withdrawing carbonyls on A3 result in the H atoms (forming the hydrogen bonds) being more electron deficient than in A2. Hence, much stronger H-bonds form in A3 than in A2. For A1, the extra ring may contribute to the stabilization energy of the complex.

Also, a comparison between the interaction energies of receptor-CO_2 complexes between ωB97X-D3/aug-cc-pVTZ and RI-MP2/aug-cc-pVTZ was carried out. We observed that the ωB97X-D3/aug-cc-pVTZ calculated interaction energies yielded reasonable results, approaching the accuracy of RI-MP2/aug-cc-pVTZ for all receptor-CO_2 complexes (Table 2.1).

In the case of fluorene-receptor complexes, their calculated interaction energies are higher than those of the receptor-CO_2 complexes (Table 2.1). The highest reactivity among the fluorene-receptor complexes was observed for the complex with receptor A3, presenting an interaction energy of -5.75 kcal/mol for DA3-CO_2 and TA3-CO_2 complexes. In general, for receptor A3, the interaction energies increase from the monomer to the trimer, which is different for receptors A1 and A2.

Table 2.2 Natural bond orbital (NBO) charge distributions for receptor-complexes in the ground state and excited state in the gas (aqueous) phase

	Ground State			**Excited State**		
Receptors	**1**	**2**	**3**	**1**	**2**	**3**
			Receptor-Complexes			
A	0.008	-0.002	-0.013	0.011	0.002	-0.011
	(0.011)	(-0.002)	(-0.017)	(0.015)	(0.003)	(-0.015)
CO_2	-0.008	0.002	0.013	-0.011	-0.002	0.011
	(-0.011)	(0.002)	(0.017)	(-0.015)	(-0.003)	(0.015)

Table 2.3 Natural bond orbital (NBO) charge distributions for monomer-complexes in the ground state and excited state in the gas (aqueous) phase

	Ground State			**Excited State**		
Receptors	**1**	**2**	**3**	**1**	**2**	**3**
M	0.010	0.011	0.035	0.062	0.066	**0.212**
	(0.043)	(0.049)	(0.074)	**(0.298)**	**(0.146)**	**(0.461)**
A	-0.003	-0.012	-0.046	-0.054	-0.066	**-0.223**
	(0.499)	**(0.485)**	**(0.399)**	**(0.258)**	**(0.124)**	(0.021)
CO_2	-0.008	0.000	0.011	-0.008	0.000	0.011
	(-0.542)	**(-0.534)**	**(-0.473)**	**(-0.556)**	**(-0.270)**	**(-0.482)**

Table 2.4 Natural bond orbital (NBO) charge distributions for dimer-complexes in the ground state and excited state in the gas (aqueous) phase

	Ground State			**Excited State**		
Receptors	**1**	**2**	**3**	**1**	**2**	**3**
D	0.004	0.013	0.033	0.009	0.038	**0.112**
	(0.021)	(0.050)	(0.075)	(0.107)	**(0.167)**	**(0.344)**
A	0.003	-0.013	-0.045	-0.001	-0.038	**-0.124**
	(0.250)	**(0.485)**	**(0.399)**	**(0.453)**	**(0.371)**	**(0.136)**
CO_2	-0.007	0.001	0.012	-0.008	0.000	0.012
	(-0.271)	**(-0.535)**	**(-0.474)**	**(-0.560)**	**(-0.538)**	**(-0.480)**

Table 2.5 Natural bond orbital (NBO) charge distributions for trimer-complexes in the ground state and excited state in the gas (aqueous) phase

	Ground State			**Excited State**		
Receptors	**1**	**2**	**3**	**1**	**2**	**3**
T	0.010	0.013	**-0.578**	0.017	0.022	**-0.549**
	(0.015)	(0.016)	**(-0.568)**	(0.024)	(0.027)	**(-0.545)**
A	-0.003	-0.013	**0.566**	-0.010	-0.023	**0.537**
	(-0.010)	(-0.014)	**(0.556)**	(-0.019)	(-0.025)	**(0.533)**
CO_2	-0.007	0.000	0.012	-0.007	0.000	0.012
	(-0.005)	(-0.002)	(0.012)	(-0.005)	(-0.002)	(0.012)

2.4.3 Natural bond orbital analysis (NBO)

NBO analysis is used to determine the closest Lewis structure for a molecule. A useful aspect of the NBO method is that it gives information about interactions in both filled and virtual orbital spaces that could enhance the analysis of intra- and intermolecular interactions.[49] Also, from the NBO analysis, charge transfer or conjugative interaction between receptors and CO_2 are obtained so as to describe the migration of electrons, which can help elucidate the sensing mechanism. Therefore, the amounts of charge transfer between the receptors and analyte were calculated by NBO (Q_{NBO}) charge analysis. The Q_{NBO} values for the ground and for the first bright excited states (see Section 2.44) obtained from the receptors and fluorene-receptor complexes are tabulated in Table 2.2 – 2.5. As shown in Table 2.2, the charges of CO_2 in the receptor complexes were almost the same in both the gas phase and in the aqueous phase.

For the fluorene-receptor complexes, the charges were separated into three components: fluorene (monomer, dimer, and trimer), receptor (A1, A2, and A3), and CO_2 (Tables 2.3-2.5). The amount of charge transfer to CO_2 in the gas phase calculations is almost the same from the monomer-receptor to the trimer-receptor complexes in both the ground and excited state. However, they differ in the aqueous phase. For the ground state complexes, the amount of charge migration to the CO_2 decreased in the aqueous phase from -0.542 to -0.005 (A1), -0.534 to -0.002 (A2), and -0.473 to 0.012 (A3) based on the calculated Q_{NBO} for the MA-CO_2 to TA-CO_2 complexes. Monomer and dimer show oligomer to receptor charge transfer in the excited state in the aqueous phase. The amount of charge transfer to analyte was largest in dimer-receptor complexes and was smallest in trimer-receptor complexes for the excited state. The decrease in charge transfer on the

analyte in the trimer-receptor complexes can be attributed to the higher delocalization of electrons in the larger π-conjugated system. For example, in TA3, the trimer has the greatest amount of charge (-0.568) as compared to CO_2 (0.012). This has also been observed in a study by Ariyageadsakul et al.,[57] where polyaniline emeraldine (PANI ES) was used as a gas sensor for detection of toxic carbonyl species. The authors observed that an increase in the PANI ES chain length resulted in a decrease in the amount of charge transfer to the analytes.

According to the charge analysis, it can be deduced that the large negative charge values on the analyte are indicative of the transfer of electrons from the fluorene-receptor to CO_2, explaining the deformation of the CO_2 bond angle and a decrease in bond distance for the monomer- and dimer-receptor complexes in the aqueous phase.

2.4.4 Electronic excitation energies

2.4.4.1 Choice of functional

Theoretical and computational modeling has proven to be a useful tool for elucidating the structural and electronic properties of organic molecules by providing in-depth understanding as well as an efficient means of designing new compounds. For an accurate description of the excited state properties of π-conjugated systems with TDDFT, the choice of functional is decisive. Thus, to select a suitable functional for describing our excited states, five different functionals (B3LYP,[58] MPW1PW91,[59] PBE0,[60] ωB97X-D,[61] and CAM-B3LYP[62]) were selected and compared with the wave function method equation-of-motion coupled-cluster singles and doubles, EOM-CCSD. In this work, the test calculations were carried out on two small molecules, DMAP and receptor A2. Table

2.6 shows the data for the most intense excited states of these molecules. From our calculations, all five functionals predicted the right symmetry state of the excited state (13 A" for DMAP and 17 A" for A2). The long-range corrected functionals (ωB97X-D and CAM-B3LYP) produced results that are in good agreement with EOM-CCSD, with the hybrid functionals yielding lower values. Of these functionals, ωB97X-D was selected to delineate the lowest lying excited states of fluorene-receptors and its interaction with carbon dioxide.

2.4.4.2 Vertical excitation energies

To elucidate the sensing ability of fluorene-receptors and receptor molecules based on the optical determination, TD-ωB97X-D with the def2-SVPD basis[47] was employed to simulate their transition energies. The computed excitation energies (E_{ex}) and oscillator strengths of these complexes are reported. Table 2.7 shows the first bright state in both gas and aqueous environments for the receptor and fluorene-receptor molecules with and without the presence of the CO_2 analyte. The solvent effect has been shown to affect the electronic excited state properties of molecules more than the ground state properties. Hence to capture solvent effects, LR-PCM/TDDFT [54,55] was employed.

From Table 2.7, the calculated excitation energies for the receptors A1, A2, and A3 are 4.63 (4.41), 4.78 (4.57), and 4.82 (4.78) eV; while that of only the fluorene monomer, dimer and trimer are 4.85 (4.80), 4.34 (4.24), and 4.13 (4.02) eV respectively in the gas (aqueous) phase. For the fluorene molecules, we observe a decrease in excitation energy as the number of repeating units increases. Upon linking the receptor and fluorene molecules to form a sensor, the calculated excitation energy decreases generally: receptors > monomer-receptors > trimer-receptors. In the monomer-receptors,

the excitation energies changes from 4.85 eV (only monomer) to 4.69 (MA1), 4.64 (MA2), and 4.50 eV (MA3).

By comparing the bare receptor sensors (A1, A2, and A3) with the CO_2 complexes, the change in transition energies is very minimal in both gas and solvent. According to Table 2.7, the change in transition energies are 0.05 (0.01), 0.07 (0.01), and 0.06 (0.07) for A1, A2, and A3 respectively for the gas (solvent) phase. For the monomer-receptors, the change in transition energies is all red-shifted and significant in the solvent upon binding to the analyte, CO_2. The largest redshift, 0.32 eV, was observed for MA3, while such shift decreased to 0.17 and 0.15 eV for MA2 and MA1 respectively in the aqueous phase. The amount of redshift tends to decrease significantly with an increase in the number of repeating units. In the gas phase, the change in transition energies upon CO_2 binding for the fluorene-receptors are minimal.

To describe relative strength of electronic transitions, the oscillator strength is used, which corresponds to absorbance.[57,63] From our results, the intensity tends to increase upon analyte binding in both gas and aqueous solution. Also, the intensities were higher in the presence of water for all molecules than in the gas phase. Previous studies have shown that LR-PCM calculations tend to overestimate the effect of solvent on intensities.[64,65]

2.4.4.3 Electron attachment/detachment density plots

To help understand the nature of electronic excitations, we performed attachment/detachment density calculations. The attachment/detachment density plots[51] pictorially represent the hole and particle densities of an electronic transition and thus can be used to characterize the excitations. Figures 2.8-2.11 show the attachment/detachment

densities for the most intense excitations of the complexes in the aqueous solution. The detachment densities are placed on the left of the arrow, and the attachment densities are on the right of the arrow. Here we see that for attachment densities of the monomer and dimer-receptor complexes, the electron densities are located on the receptor but not so for the trimer. This indicates that the electronic excitations in the trimer-receptor complexes are mainly due to transitions from the trimer, while for the monomer and dimer complexes there is a contribution from the receptors.

Table 2.6 Calculated vertical excitation energies (in eV) with the most intense strength for DMAP and Analogue 2

	Dmap			**Analogue 2**		
Method	**State**	**Excitation Energy**	**Oscillator Strength**	**State**	**Excitation Energy**	**Oscillator Strength**
TD-B3LYP	13 A"	6.63	0.360	17 A'	6.52	0.399
TD-PBE0	13 A"	6.76	0.418	17 A'	6.72	0.284
TD-MPW1PW91	13 A"	6.75	0.463	17 A'	6.70	0.328
TD-ωB97X-D	13 A"	6.85	0.549	17 A'	6.80	0.453
TD-CAM-B3LYP	13 A"	6.83	0.574	17 A'	6.69	0.258
EOM-CCSD	13 A"	7.14	0.499	17 A'	6.90	0.320

Table 2.7 Calculated vertical excitation energies (E) in eV, oscillator strength (f), and ΔEex of (fluorene)-receptor before and after interacting with CO2 in the gas and aqueous solution by TD-ωB97X-D/def2-SVPD.

	Vacuum			Aqueous		
	E_{rec} (*f*)	E_{comp} (*f*)	ΔE[a]	E_{rec} (*f*)	E_{comp} (*f*)	ΔE[a]
Receptor complexes						
A1	4.63 (0.103)	4.58 (0.104)	-0.05	4.41 (0.155)	4.42 (0.150)	0.01
A2	4.78 (0.130)	4.71 (0.125)	-0.07	4.57 (0.196)	4.56 (0.184)	-0.01
A3	4.82 (0.288)	4.76 (0.284)	-0.06	4.78 (0.387)	4.71 (0.369)	-0.07
Monomer-receptor complexes						
Monomer	4.85 (0.276)			4.80 (0.445)		
MA1	4.69 (0.675)	4.68 (0.719)	-0.01	4.60 (0.920)	4.45 (0.958)	-0.15
MA2	4.64 (0.774)	4.65 (0.788)	0.01	4.51 (1.046)	4.34 (1.186)	-0.17
MA3	4.50 (0.922)	4.49 (0.949)	-0.01	4.42 (1.104)	4.10 (1.170)	-0.32
Dimer-receptor complexes						
Dimer	4.34 (1.460)			4.24 (1.719)		
DA1	4.36 (1.174)	4.30 (1.840)	-0.06	4.13 (2.120)	4.20 (1.201)	0.07
DA2	4.22 (1.937)	4.24 (1.975)	0.02	4.12 (2.201)	4.04 (2.295)	-0.08
DA3	4.13 (2.035)	4.20 (2.038)	0.07	4.04 (2.256)	3.88 (2.150)	- 0.06
Trimer-receptor complexes						
Trimer	4.13 (2.555)			4.02 (2.815)		
TA1	4.11 (2.914)	4.07 (3.014)	-0.04	3.96 (3.167)	4.00 (3.206)	0.04
TA2	4.05 (2.985)	4.07 (3.080)	0.02	3.93 (3.209)	3.98 (3.285)	0.05
TA3	4.02 (3.214)	4.05 (3.147)	0.03	3.93 (3.425)	3.96 (3.310)	0.03

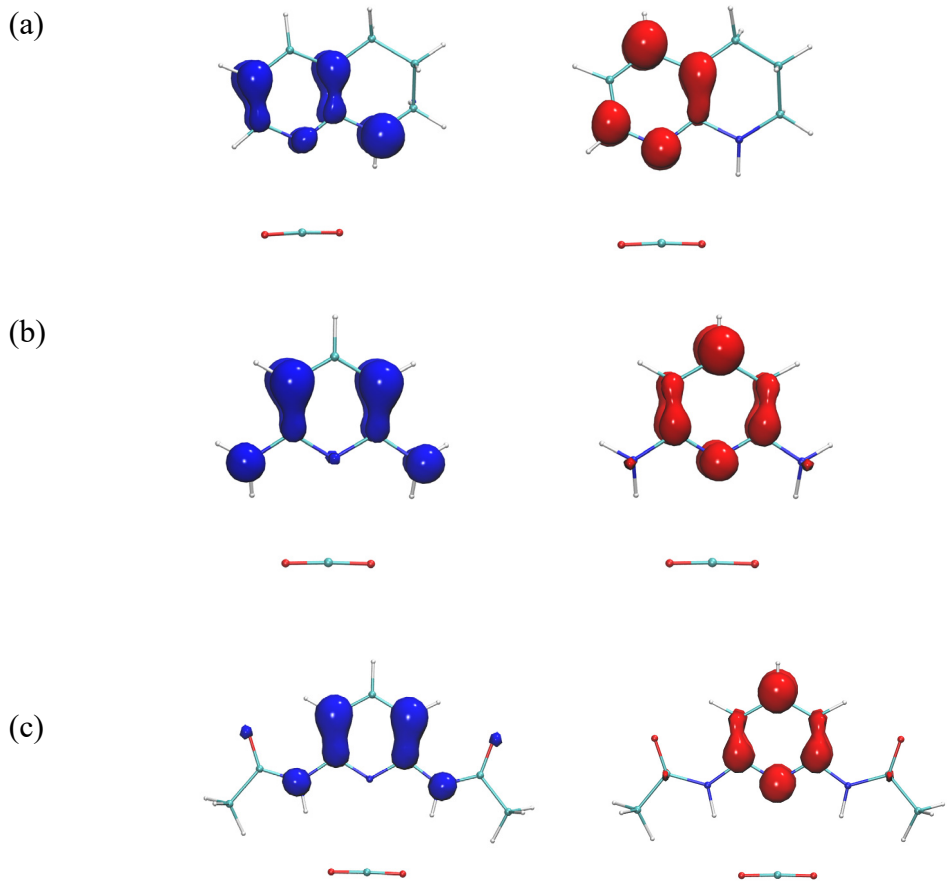

Figure 2.8 Attachment/detachment density plots of receptor-CO_2 complexes. (a) A1-CO_2 (b) A2-CO_2 (c) A3-CO_2

Images on the left (in blue) are the detachment densities and on the right (red) are the attachment densities

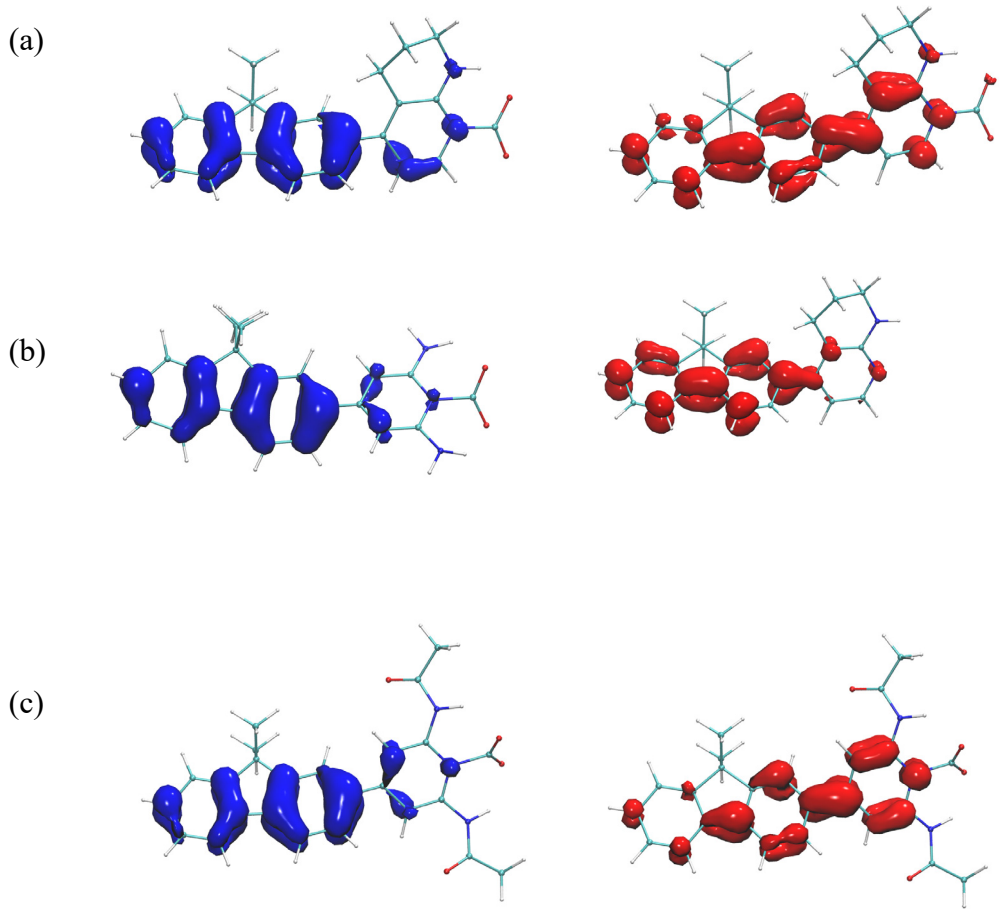

Figure 2.9 Attachment/detachment density plots of monomer-receptor-CO_2 complexes. (a) MA1-CO_2 (b) MA2-CO_2 (c) MA3-CO_2

Images on the left (in blue) are the detachment densities and on the right (red) are the attachment densities

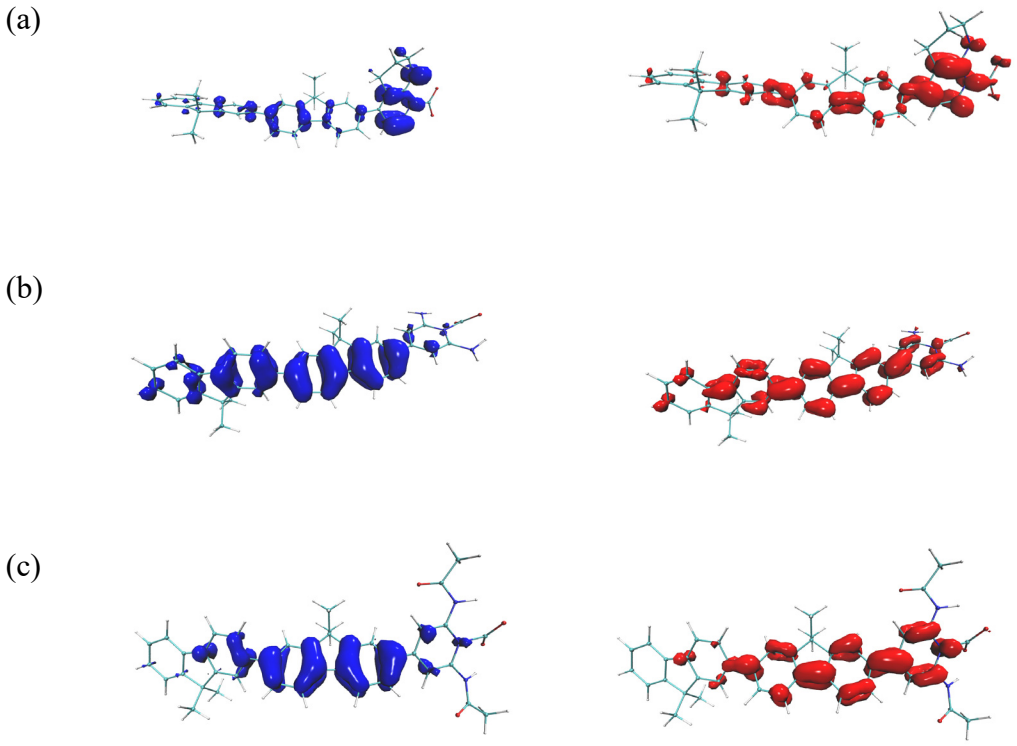

Figure 2.10 Attachment/detachment density plots of dimer-receptor-CO_2 complexes. (a) DA1-CO_2 (b) DA2-CO_2 (c) DA3-CO_2

Images on the left (in blue) are the detachment densities and on the right (red) are the attachment densities

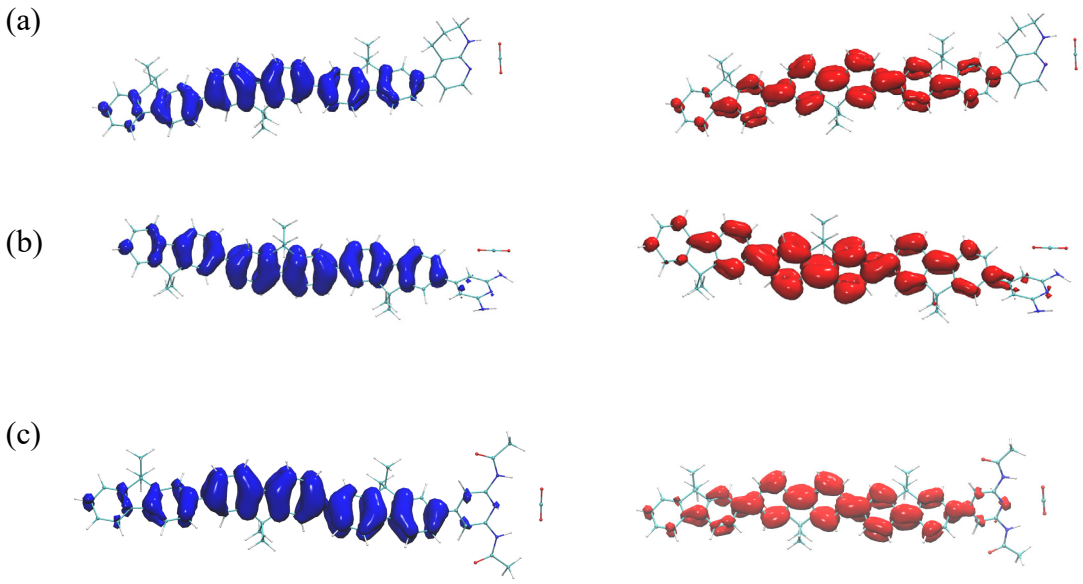

Figure 2.11 Attachment/detachment density plots of trimer-receptor-CO_2 complexes. (a) TA1-CO_2 (b) TA2-CO_2 (c) TA3-CO_2

Images on the left (in blue) are the detachment densities and on the right (red) are the attachment densities

2.5 Conclusion

Theoretical calculations have been carried out to describe the interactions of carbon dioxide with fluorene/receptor molecules. Density functional theory was employed to describe the nature of the interactions between CO_2 and the receptor molecules. To delineate the electronic properties and charge transfer within complexes, TDDFT and NBO analyses were employed. From this study we can draw the following conclusions:

(a) The interactions between receptor molecules and CO_2 occur via Lewis acid-Lewis base interactions, and weak hydrogen bonding of the negatively charged oxygen atoms of CO_2 with the proximal hydrogens of the receptor molecules provides further stabilization of the complexes. From the binding selectivity study, the calculated interaction energies of the receptor-CO_2 complexes are -5.41, -5.27, and -5.75 kcal/mol in A1, A2, and A3 respectively.

(b) The NBO charge analysis indicates the transfer of electrons from fluorene-receptor molecules to the CO_2 analyte in the aqueous phase. The amount of charge transfer to the CO_2 decreases with increase in oligomer chain length due to the high delocalization of electrons in the longer π-conjugated systems. For the receptor-CO_2 complexes, we observed that the amount of charge transfer to the analyte is minimal.

(c) The TDDFT electronic absorption studies of the complexes suggest that the receptor molecules cannot be used as stand-alone sensors for CO_2 but the fluorene-receptor molecules, especially the monomer, can be used. The monomer-receptor complexes showed remarkable redshifts in their absorption spectra; the

effect was much stronger in water than in the gas phase.

(d) Comparison of the attachment/detachment density plots help explain the nature of the electronic excitations upon CO_2 binding. The attachment/detachment density plots of the fluorene-receptor complexes reveal that there is a decrease in electron density on the receptors upon CO_2 binding with an increase in chain length. This is an indication of the receptor contributing to the most intense state upon CO_2 binding in the monomer and dimer complexes.

CHAPTER III

SUMMARY AND OUTLOOK

The rising level of carbon dioxide concentration in the atmosphere is a major concern for various stakeholders. Of primary concern is ocean acidification due to the uptake of CO_2 released by human activities with a major impact on marine ecosystems. The use of chemical sensors for monitoring various gases and analytes has proven to be a valuable tool. The main goal of this research is to evaluate the use of various polymer-receptors for CO_2 monitoring.

In this thesis, we presented the binding energies and structural and optical properties of CO_2 receptors complexed with fluorene oligomers as a sensor. From our results, the interactions between CO_2 and the receptors are weak: Lewis acid-Lewis base interactions along with weak hydrogen bonds stabilize the complexes. The calculated excitation energies reveal a change in transition energies upon CO_2 binding. The monomer-receptor complexes show remarkable redshifts in their absorption spectra, which decrease on moving to dimer and trimer-receptor complexes. This effect is much stronger in water than in the gas phase.

In addition, natural bond orbital (NBO) charge analysis and electron attachment/detachment density plots were carried out to analyze the nature of electronic excitations. Both analyses revealed a decrease in electron density on the receptors as the

oligomer chain increases. Overall, a fluorene monomer complexed with receptor A3 will be the most suitable sensor for CO_2 monitoring.

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APPENDIX A

SUPPORTING INFORMATION

This section contains

1. RI-MP2/cc-pVTZ optimized XYZ coordinates (in Angstroms) of receptor and receptor-CO_2 molecules

2. ωB97X-D3/def2-TZVP optimized XYZ coordinates (in Angstroms) of fluorene-receptors and fluorene-recepotor-CO_2 molecules.

A.1. XYZ coordinates for receptors and receptor complexes

A1 in gas phase

C	-0.1210866358	-0.7289245392	0.0414580267
C	-2.5300869581	-0.6455287655	0.0076249767
N	-1.2699485066	1.4010567539	-0.0535970363
C	-2.4330186054	0.7393983793	-0.0363127527
C	-0.1417129872	0.6790114035	-0.0248989249
C	-1.3476137348	-1.3800645569	0.0482707501
H	-3.3240558967	1.3547989848	-0.0586602299
H	-1.3717542369	-2.4626662881	0.0878285409
H	-3.4958038173	-1.1288667343	0.0137847037
C	1.1864555416	-1.4751009014	0.1147838857
H	1.3674109380	-1.7774645600	1.1496276850
H	1.1176229062	-2.3921687717	-0.4716141122
C	2.3479429252	-0.6111664011	-0.3655794101
H	3.2993249842	-1.0888373709	-0.1336792890
H	2.2920579564	-0.4758128153	-1.4463024899
C	2.2728279751	0.7569858543	0.2949565034
H	2.3409378174	0.6380909117	1.3842126755
H	3.1032102261	1.3846533323	-0.0239721664
N	1.0364423120	1.3946324757	-0.1104443436
H	0.9132618323	2.3687023450	0.1204949829

A1 in aqueous phase

C	-0.1168183686	-0.7299833930	0.0523517861
C	-2.5286035050	-0.6459641932	0.0131717120
N	-1.2633654977	1.4163417279	-0.0655054706
C	-2.4337429950	0.7385392821	-0.0450861937
C	-0.1302042125	0.6785991265	-0.0263060455
C	-1.3432077897	-1.3824085652	0.0629133913
H	-3.3209970606	1.3630692617	-0.0789006704
H	-1.3678875394	-2.4584450957	0.1106999501
H	-3.4948210842	-1.1237495313	0.0211595199
C	1.1917068131	-1.4774211060	0.1277330234
H	1.3743027706	-1.7594236416	1.1618402119

H	1.1119391112	-2.3948430560	-0.4464061076
C	2.3509943327	-0.6210442945	-0.3781627587
H	3.2967599784	-1.0985759553	-0.1549243875
H	2.2773524364	-0.4994854873	-1.4582145701
C	2.2934491008	0.7572503951	0.2670611079
H	2.3753955271	0.6594565051	1.3504584116
H	3.1064815923	1.3805956523	-0.0827996980
N	1.0438716869	1.3910162567	-0.1222388185
H	0.9297330652	2.3768501447	0.0546473615

A1-CO_2 in gas phase

C	1.5578195982	0.7258969785	-0.0678333784
C	0.2030060353	2.7211086187	-0.0291705612
N	-0.8479353161	0.5677706429	0.1309939203
C	-0.9136628310	1.9040379187	0.0816662444
C	0.3613231970	-0.0088637436	0.0661440949
C	1.4525282337	2.1095665752	-0.1050319212
H	-1.9104547840	2.3246750644	0.1342646963
H	2.3530069285	2.7055229293	-0.1957036570
H	0.0969805667	3.7953473328	-0.0581947759
C	2.8823793590	0.0153968255	-0.1737872306
H	3.1870133462	-0.0191196874	-1.2231241933
H	3.6464299460	0.5859059742	0.3556717759
C	2.7930098606	-1.4067772954	0.3696793309
H	3.6976027276	-1.9642396223	0.1289286759
H	2.6872062716	-1.3865340869	1.4550458527
C	1.5760793431	-2.1022406022	-0.2210471901
H	1.6788546262	-2.1479249690	-1.3130010869
H	1.4993601455	-3.1236552191	0.1478146261
N	0.3871938798	-1.3813203019	0.1853767411
H	-0.5091450229	-1.8124956696	0.0145097305
C	-3.2947051899	-0.7657725937	-0.0490897267
O	-3.8660967374	0.2446216036	0.0768338112
O	-2.7879810428	-1.8137997995	-0.1834374564

A1-CO_2 in aqueous phase

C	1.5756440059	0.7091494788	-0.0566120968
C	0.2303233813	2.7155527106	-0.0472505131
N	-0.8451350293	0.5585099925	0.0531673952
C	-0.8951559757	1.9045998748	0.0178499569
C	0.3717040034	-0.0227731953	0.0223346046
C	1.4808157366	2.0948597123	-0.0841336176
H	-1.8954860073	2.3250739067	0.0482484922
H	2.3818737438	2.6827548276	-0.1330720594
H	0.1285626898	3.7880078831	-0.0672810023

C	2.9024661589	-0.0073810942	-0.1119096115
H	3.2481348152	-0.0263123584	-1.1422136648
H	3.6336590753	0.5514140468	0.4625409362
C	2.7826790408	-1.4381662683	0.4104149532
H	3.6894277832	-1.9918861116	0.2019694786
H	2.6306282190	-1.4271310251	1.4887436656
C	1.5873178209	-2.1243676133	-0.2370197228
H	1.7223546699	-2.1550746888	-1.3190254579
H	1.4832379309	-3.1403361865	0.1232948124
N	0.3857843915	-1.3943288919	0.1335923683
H	-0.5114824648	-1.8226611983	-0.0405725576
C	-3.2927802104	-0.7181256952	0.0218788812
O	-3.8498232542	0.3015805701	0.1729297755
O	-2.8174722766	-1.7785753134	-0.1334969222

A2 in gas phase

H	0.0198294289	2.8848046741	0.0000000000
C	0.0090763370	1.8031706073	0.0000000000
C	-0.0124631089	-0.2872387388	1.1483629730
C	-0.0124631089	-0.2872387388	-1.1483629730
N	-0.0063524581	-0.9718184981	0.0000000000
C	-0.0029742486	1.1091875485	-1.2014985180
C	-0.0029742486	1.1091875485	1.2014985180
H	-0.0119753802	1.6243702248	-2.1509509847
H	-0.0119753802	1.6243702248	2.1509509847
N	-0.0832893680	-1.0514176539	-2.3061524841
H	0.1992413558	-2.0060469254	-2.1481427923
H	0.3599514069	-0.6404366481	-3.1110875946
N	-0.0832893680	-1.0514176539	2.3061524841
H	0.1992413558	-2.0060469254	2.1481427923
H	0.3599514069	-0.6404366481	3.1110875946

A2 in aqueous phase

H	-0.0302923591	2.8965196146	0.0000000000
C	-0.0142151942	1.8193230304	0.0000000000
C	0.0184729542	-0.2719701480	-1.1551820635
C	0.0184729561	-0.2719701493	1.1551820613
N	0.0154420091	-0.9693865477	0.0000000000
C	0.0013009839	1.1262417139	1.2056337125
C	0.0013009833	1.1262417152	-1.2056337132
H	0.0090290612	1.6407745305	2.1505623322
H	0.0090290602	1.6407745328	-2.1505623321
N	0.0952419234	-1.0431086110	2.3059045731
H	-0.1927233213	-1.9965356412	2.1570083541
H	-0.2803188027	-0.6248211035	3.1334592386

N	0.0952419198	-1.0431086148	-2.3059045720
H	-0.1927233238	-1.9965356455	-2.1570083540
H	-0.2803187970	-0.6248211083	-3.1334592422

A2-CO_2 in gas phase

H	-3.9300020263	0.4079685134	0.0000000000
C	-2.8625732429	0.2325502371	0.0000000000
C	-0.7989626943	-0.1075138383	-1.1503958556
C	-0.7989626943	-0.1075138383	1.1503958556
N	-0.1181702986	-0.2032815180	0.0000000000
C	-2.1781681560	0.1145370220	1.2003529531
C	-2.1781681560	0.1145370220	-1.2003529531
H	-2.6881550138	0.1827068672	2.1502454124
H	-2.6881550138	0.1827068672	-2.1502454124
N	-0.0674526560	-0.2998369770	2.3116199128
H	0.9226084651	-0.1575659486	2.1893826127
H	-0.4376005454	0.1605871321	3.1261664988
N	-0.0674526560	-0.2998369770	-2.3116199128
H	0.9226084651	-0.1575659486	-2.1893826127
H	-0.4376005454	0.1605871321	-3.1261664988
C	2.8506289343	0.1425508306	0.0000000000
O	2.8796273951	0.1482446316	-1.1688002193
O	2.8796273951	0.1482446316	1.1688002193

A2-CO_2 in aqueous phase

H	-3.8718340697	0.5951314587	-0.0000000711
C	-2.8271867753	0.3332547953	-0.0000000257
C	-0.7990165692	-0.1800609621	-1.1552567915
C	-0.7990159819	-0.1800586087	1.1552566910
N	-0.1206400818	-0.3320245730	-0.0000000883
C	-2.1563763319	0.1572568563	1.2046649545
C	-2.1563765109	0.1572561551	-1.2046650051
H	-2.6594811954	0.2639771788	2.1494125584
H	-2.6594813061	0.2639768699	-2.1494125980
N	-0.0797757673	-0.4442560191	2.3120372930
H	0.9170698472	-0.3502888537	2.1878697736
H	-0.4269841609	-0.0026433462	3.1406076969
N	-0.0797757780	-0.4442559758	-2.3120375981
H	0.9170698659	-0.3502882920	-2.1878699780
H	-0.4269843005	-0.0026421371	-3.1406073277
C	2.7465067326	0.3645724072	0.0000001684
O	2.7749565076	0.3746864266	-1.1670174327
O	2.7749567936	0.3746875216	1.1670178011

A3 in gas phase

H	0.0133548802	1.9947293234	2.1630286886
C	0.0058120591	1.4964102554	1.2096958607
C	0.0058120591	1.4964102554	-1.2096958607
N	-0.0318255641	-0.5830013607	0.0000000000
C	-0.0193331635	0.1026954195	-1.1469398287
C	-0.0193331635	0.1026954195	1.1469398287
C	0.0183838880	2.1798740095	0.0000000000
H	0.0133548802	1.9947293234	-2.1630286886
H	0.0375691551	3.2609469037	0.0000000000
N	-0.0356081930	-0.7297113230	2.2714563548
N	-0.0356081930	-0.7297113230	-2.2714563548
H	-0.0503581992	-1.7096943691	-2.0370024732
H	-0.0503581992	-1.7096943691	2.0370024732
C	-0.0101381946	-0.3789705439	-3.5993324592
C	-0.0101381946	-0.3789705439	3.5993324592
O	0.0056699524	0.7741140395	-4.0000591351
O	0.0056699524	0.7741140395	4.0000591351
C	0.0322846287	-1.5624730578	-4.5372107448
H	-0.4312006467	-2.4511249139	-4.1151103675
H	1.0717834730	-1.7895875146	-4.7699949364
H	-0.4700139914	-1.2889426482	-5.4592506616
C	0.0322846287	-1.5624730578	4.5372107448
H	-0.4700139914	-1.2889426482	5.4592506616
H	1.0717834730	-1.7895875146	4.7699949364
H	-0.4312006467	-2.4511249139	4.1151103675

A3 in aqueous phase

H	0.0150042052	2.0264311905	2.1526148466
C	0.0084669949	1.5144756474	1.2065531629
C	0.0091446981	1.5130402187	-1.2053336205
N	-0.0231747489	-0.5500934523	0.0014178552
C	-0.0124413984	0.1231989533	-1.1447404620
C	-0.0130007986	0.1245152603	1.1471250503
C	0.0195651835	2.1927210953	0.0000971609
H	0.0162277083	2.0235542303	-2.1522381391
H	0.0360412789	3.2751741289	-0.0013624030
N	-0.0281695088	-0.7152258232	2.2628823525
N	-0.0271187718	-0.7159527994	-2.2619064493
H	-0.0423429113	-1.6954963107	-2.0251705977
H	-0.0433145229	-1.6944040483	2.0245993733
C	-0.0088522656	-0.3949223167	-3.5892965528
C	-0.0094398660	-0.3944938543	3.5898258249
O	0.0044834119	0.7507203546	-4.0068764206

O	0.0043370783	0.7513020590	4.0069670562
C	0.0253398649	-1.5844813460	-4.5131521420
H	-0.4240642862	-2.4714970253	-4.0714099866
H	1.0674639430	-1.8063552812	-4.7490021397
H	-0.4875502101	-1.3281630386	-5.4364319118
C	0.0254718284	-1.5846645774	4.5123998574
H	-0.4856586966	-1.3292474233	5.4368588622
H	1.0679158253	-1.8075883993	4.7457819146
H	-0.4252934414	-2.4705799714	4.0697975080

A3-CO_2 in gas phase

H	2.1625713287	-2.6178631596	0.0005136785
C	1.2086587084	-2.1206123603	0.0005171690
C	-1.2085282264	-2.1202937369	0.0025826557
N	0.0003697420	-0.0379020182	0.0023744191
C	-1.1485756155	-0.7261301188	0.0038952854
C	1.1491368398	-0.7263983517	0.0003177620
C	-0.0000127941	-2.8046362393	0.0012538309
H	-2.1625985952	-2.6172418058	0.0023681699
H	-0.0001471090	-3.8858804482	0.0008466980
N	2.2795079085	0.0964763135	-0.0014903679
N	-2.2786837320	0.0971964406	0.0064492289
H	-2.0640243301	1.0816987939	0.0136146542
H	2.0652588492	1.0811144330	-0.0076846868
C	-3.6029954986	-0.2671886582	0.0169822724
C	3.6038242918	-0.2682651368	-0.0143578649
O	-3.9972584062	-1.4228386463	0.0064934325
O	3.9977544390	-1.4239985009	-0.0041764501
C	-4.5545211163	0.9051432177	0.0684981027
H	-4.9759173697	0.9633493134	1.0705843069
H	-5.3698084832	0.7160776731	-0.6236881423
H	-4.0822353396	1.8546488745	-0.1710014924
C	4.5542651434	0.9046935491	-0.0708038036
H	4.9384724115	0.9896203594	-1.0860207231
H	5.3935883538	0.6987362470	0.5866295746
H	4.0901483745	1.8472664852	0.2089654844
C	0.0005289847	3.0185697011	-0.0011462650
O	-1.1683814733	3.0412795572	-0.0010322828
O	1.1694398991	3.0409787300	-0.0013093520

A3-CO_2 in aqueous phase

H	-0.1188679894	-2.6543874387	2.1684049023
C	-0.1136804968	-2.1507085242	1.2112283003
C	-0.1137200865	-2.1506869771	-1.2112397242

N	-0.0742325645	-0.0728187603	0.0000143825
C	-0.0844165845	-0.7565271534	-1.1489609127
C	-0.0843322399	-0.7565450255	1.1489786159
C	-0.1315218766	-2.8373565871	-0.0000120696
H	-0.1188979696	-2.6543468712	-2.1684284899
H	-0.1558477276	-3.9163411870	-0.0000228271
N	-0.0615655095	0.0783335946	2.2715306357
N	-0.0615066834	0.0783557088	-2.2715018808
H	-0.0540232293	1.0530446291	-2.0417460577
H	-0.0543515135	1.0530289261	2.0417908068
C	0.0294705820	-0.2589043712	-3.5870894028
C	0.0295842216	-0.2588979686	3.5871171395
O	0.0580136337	-1.4219469493	-4.0004410341
O	0.0583526276	-1.4219231746	4.0004990800
C	0.1254865272	0.9142178849	-4.5295227610
H	-0.2492921617	1.8292161958	-4.1054573350
H	-0.4210077042	0.6621512506	-5.4302668786
H	1.1675390089	1.0426050424	-4.7973661393
C	0.1253282496	0.9142623650	4.5295277615
H	1.1673633728	1.0429683916	4.7972847766
H	-0.4210245606	0.6620599188	5.4303184869
H	-0.2497452671	1.8291380852	4.1054626841
C	-0.0974201196	2.9747546058	-0.0000006336
O	-0.0976006078	2.9828528961	-1.1584628944
O	-0.0975733315	2.9828614933	1.1584614687

A.2. XYZ coordinates for fluorene-receptors and fluorene-receptor complexes

A. Monomer-Receptors

Monomer in gas phase

H	-1.2983970399	-2.9589170579	-0.0008849953
C	-1.6361784946	-1.9288201900	-0.0001447820
C	-2.5199029535	0.7295417628	0.0012534094
C	-0.7277580636	-0.8814681756	0.0010045969
C	-2.9930471117	-1.6373552465	-0.0007196127
C	-3.4323581473	-0.3188819527	-0.0000275309
C	-1.1675436783	0.4426156192	0.0017220769
H	-3.7169318720	-2.4438088825	-0.0019441062
H	-2.8728536096	1.7553550247	0.0014984630
C	0.7400476057	-0.8806392340	0.0007754870
C	3.4418583391	-0.3242592023	-0.0003943019
C	1.6438168964	-1.9309260802	-0.0007507114

C	1.1797534562	0.4446672300	0.0014949456
C	2.5322979138	0.7275035184	0.0009385140
C	3.0009056108	-1.6421852092	-0.0013327689
H	1.3006198264	-2.9594925445	-0.0017430347
H	2.8870819469	1.7525170323	0.0012972925
H	3.7222921473	-2.4506086525	-0.0026413598
H	4.5048848974	-0.1157086234	-0.0009345131
C	0.0030610111	1.4077164274	0.0009842546
C	-0.0084696079	2.2768206783	-1.2610519059
H	0.8703276685	2.9238558451	-1.2952072452
H	-0.8972560984	2.9115204708	-1.2811430482
H	-0.0137397086	1.6552603439	-2.1579062791
C	-0.0085654246	2.2801765277	1.2605092482
H	0.8701035863	2.9274664544	1.2927779311
H	-0.0138525654	1.6610809475	2.1590321985
H	-0.8974284276	2.9148318144	1.2786198476
H	-4.4954117676	-0.1081663954	-0.0007502016

Monomer in aqueous phase

H	7.5498978381	5.0177658714	3.3099284875
C	6.8668510315	5.2525404922	2.5011371912
C	5.0945440286	5.8525017305	0.4086634824
C	7.2527541492	6.0861374625	1.4606733322
C	5.5836616188	4.7191233728	2.4869273149
C	4.7044860777	5.0162676008	1.4499243089
C	6.3713979662	6.3850420584	0.4190876630
H	5.2635292357	4.0641908569	3.2890133725
H	4.4041954248	6.0780518734	-0.3974768833
C	8.5216732490	6.7802536558	1.2011276378
C	10.6461189536	8.2637264684	0.2489470965
C	9.7056240099	6.7992584584	1.9229575448
C	8.3952788384	7.4958059756	0.0072125388
C	9.4564546765	8.2414966319	-0.4733253656
C	10.7695089252	7.5482436512	1.4360322911
H	9.8013574736	6.2400734782	2.8470165269
H	9.3693423833	8.8004019226	-1.3991670316
H	11.7035896628	7.5750974002	1.9848550908
H	11.4855372782	8.8433458046	-0.1170446243
C	7.0148865971	7.3066068433	-0.6020491908
C	7.0963893536	6.6371582123	-1.9801134747
H	7.6197186945	7.2834257934	-2.6880744938
H	6.0934785628	6.4499933410	-2.3706985600
H	7.6264411006	5.6843869535	-1.9241212246
C	6.2545574587	8.6337777874	-0.7110013679
H	6.7670857849	9.3125304071	-1.3960199586

H	6.1719805904	9.1203889854	0.2626286591
H	5.2468657000	8.4617428771	-1.0961500296
H	3.7072356673	4.5909798426	1.4523572685

MA1 in gas phase

C	3.0461327884	-0.0310233641	-0.0960802797
C	2.7812146913	2.1494910437	0.8754206795
N	4.9655440774	1.2038138305	0.7078411710
C	4.1453966059	2.1848779123	1.0653844106
C	4.4303474318	0.1293007152	0.1331203061
C	2.2164869725	1.0142496061	0.2868280217
H	4.6130467450	3.0458969030	1.5336552498
H	2.1552300587	2.9720197014	1.1954192793
C	2.5469440161	-1.2902290545	-0.7696181231
H	2.1722092366	-1.9925761110	-0.0169388738
H	1.6949151021	-1.0547874759	-1.4101753960
C	3.6446138706	-1.9762477312	-1.5751079737
H	3.3039944758	-2.9534940627	-1.9223877230
H	3.8892644272	-1.3792753151	-2.4577343177
C	4.8949723319	-2.1324547460	-0.7253465738
H	4.6862451533	-2.8124383415	0.1137967917
H	5.7038668465	-2.5761031477	-1.3087231584
N	5.3183352495	-0.8320157765	-0.2674306844
H	6.2558599107	-0.6994688862	0.0675420045
H	-1.6992341157	2.7655084602	-1.4700775800
C	-1.2404051970	1.9733001878	-0.8897592257
C	-0.0332182767	-0.0649564843	0.5956627868
C	-1.9997536763	0.9381433187	-0.3705300900
C	0.1272578525	1.9797649804	-0.6633213815
C	0.7455890952	0.9672366951	0.0705243179
C	-1.3954566271	-0.0776214430	0.3728937677
H	0.7368294352	2.7754597851	-1.0749838974
H	0.4382484143	-0.8460818036	1.1823024112
C	-3.4390957467	0.6588613115	-0.4551157740
C	-6.0141585016	-0.3367845700	-0.3138865286
C	-4.4667329559	1.3466008922	-1.0835094067
C	-3.6968027964	-0.5237899498	0.2398235044
C	-4.9832739510	-1.0250880515	0.3143121180
C	-5.7563713669	0.8394213978	-1.0078174970
H	-4.2727485599	2.2632790844	-1.6283314813
H	-5.1939771517	-1.9438046752	0.8514886802
H	-6.5705173302	1.3628718140	-1.4949364904
H	-7.0265357534	-0.7201764676	-0.2640605473
C	-2.4221513836	-1.1054733719	0.8259401568

C	-2.1308547171	-2.4871658661	0.2269251055
H	-2.9145404793	-3.1967428010	0.5021567982
H	-1.1794614744	-2.8774435665	0.5950195202
H	-2.0846529904	-2.4380667721	-0.8621308038
C	-2.5054539247	-1.1947938772	2.3533024113
H	-3.2952618910	-1.8874442066	2.6531627782
H	-2.7246468185	-0.2193009310	2.7894640883
H	-1.5644235193	-1.5565002320	2.7728286474

MA1 in aqueous phase

C	1.9984064622	2.3930424722	-0.2771554988
C	1.5244543446	3.6831189164	1.6978051478
N	-0.1639558986	2.2491212072	0.8077119057
C	0.2652935293	3.1309291241	1.7101622205
C	0.6828962067	1.8810976924	-0.1572375896
C	2.4100943789	3.3142353430	0.6756839606
H	-0.4497504979	3.4101136402	2.4786576159
H	1.8150194463	4.4085740696	2.4462343139
C	2.8781951923	1.8997986709	-1.4045529722
H	2.8549826702	2.6158274903	-2.2321395474
H	3.9161775649	1.8531235705	-1.0702160784
C	2.4248123469	0.5408074366	-1.9254422465
H	2.9833322110	0.2782656251	-2.8251581724
H	2.6178129486	-0.2340864927	-1.1780505144
C	0.9386357622	0.5750318821	-2.2320583894
H	0.7451450217	1.2848777266	-3.0474092831
H	0.5843760380	-0.4036383654	-2.5581746332
N	0.2180505986	0.9416164784	-1.0311320809
H	-0.7713191139	0.7646631642	-0.9899457037
H	6.4345266996	4.5185375282	2.6619269788
C	5.8139898720	4.5465535272	1.7733280130
C	4.1953810698	4.6032262988	-0.5105064532
C	6.2397725458	5.1947992322	0.6231718479
C	4.5710579529	3.9280611583	1.7715412965
C	3.7551305606	3.9463211925	0.6384058072
C	5.4303063649	5.2183261436	-0.5137744544
H	4.2256194513	3.4141649569	2.6614289433
H	3.5611056745	4.6386510674	-1.3894686243
C	7.4749942331	5.9304352624	0.3205967657
C	9.5570136637	7.3904045216	-0.7576576650
C	8.5847543243	6.2019533202	1.1070900162
C	7.4020748623	6.3853936756	-0.9995036921
C	8.4424463900	7.1155837581	-1.5442327220
C	9.6268564884	6.9372943185	0.5563234164
H	8.6391100044	5.8493370333	2.1309681518

H	8.3947754918	7.4717560906	-2.5678853798
H	10.5017905258	7.1614045919	1.1551956269
H	10.3788091844	7.9628358798	-1.1717324270
C	6.0964052958	5.9645729862	-1.6545684243
C	6.3391544994	5.0318213668	-2.8488596706
H	6.8741831259	5.5579595974	-3.6422959373
H	5.3872219822	4.6822358046	-3.2554700294
H	6.9264453804	4.1601383265	-2.5537707740
C	5.2623160807	7.1725990672	-2.0969337339
H	5.7839686190	7.7314677592	-2.8767406571
H	5.0673993667	7.8448214524	-1.2593360412
H	4.3035920782	6.8414794307	-2.5027686329

MA1-CO_2 in gas phase

C	2.1273467017	-0.4265883918	-0.2580500677
C	2.1242029270	1.8726956347	0.4396142955
N	4.1986716094	0.7107593739	0.2573910199
C	3.4950082453	1.8036270219	0.5365318230
C	3.5348059181	-0.3762586784	-0.1353545390
C	1.4219803142	0.7315668537	0.0351442595
H	4.0731196175	2.6659236271	0.8544236823
H	1.5963021998	2.7834730515	0.6889771964
C	1.4813924792	-1.7046093962	-0.7432985384
H	1.1376146269	-2.2988945664	0.1106657217
H	0.5894891381	-1.4712818200	-1.3272463226
C	2.4503228529	-2.5466465811	-1.5654286234
H	2.0048097969	-3.5147939954	-1.8014788430
H	2.6699629801	-2.0445439375	-2.5115087699
C	3.7455441073	-2.7459227671	-0.7964051660
H	3.5514602357	-3.3554895571	0.0977541794
H	4.4753025740	-3.2855731937	-1.4027600933
N	4.2998665533	-1.4603568102	-0.4496102412
H	5.2812944800	-1.3702092833	-0.2538738159
H	-2.4206010922	2.6411860741	-1.7132431452
C	-2.0000499343	1.8748056142	-1.0724194263
C	-0.8913117626	-0.1038144047	0.5625232543
C	-2.8143017647	0.9616362884	-0.4237218242
C	-0.6270648006	1.7865210794	-0.9034064038
C	-0.0576748344	0.8004057451	-0.0973717420
C	-2.2590877563	-0.0241213987	0.3944431821
H	0.0239580974	2.4813220792	-1.4207148446
H	-0.4571306635	-0.8625423211	1.2046060594
C	-4.2727506615	0.7899663941	-0.4342017812
C	-6.9067029003	0.0114034683	-0.1227046844

C	-5.2697209133	1.4944698051	-1.0927120401
C	-4.5903623877	-0.3012770925	0.3759879043
C	-5.9065356608	-0.6937886171	0.5356358933
C	-6.5894012419	1.0967280836	-0.9308206874
H	-5.0291369186	2.3398661572	-1.7269639209
H	-6.1639156782	-1.5417895076	1.1614713645
H	-7.3806411409	1.6342211099	-1.4399022565
H	-7.9418982729	-0.2877288621	-0.0075043551
C	-3.3407536008	-0.9244031299	0.9731960143
C	-3.1729058754	-2.3713503972	0.4917765129
H	-3.9943468149	-2.9937958710	0.8540593726
H	-2.2383842052	-2.7978139493	0.8629588028
H	-3.1650138668	-2.4210244523	-0.5982809667
C	-3.3719433803	-0.8726928455	2.5038895931
H	-4.1965703500	-1.4765710330	2.8895533752
H	-3.5055342492	0.1507822364	2.8567507848
H	-2.4433417544	-1.2641205808	2.9244325808
C	6.9776864612	0.9412257823	0.5156557393
O	6.8714368647	2.0599792125	0.7809107601
O	7.1682005015	-0.1730901843	0.2581318746

MA1-CO_2 in aqueous phase

C	1.9865520904	2.4250847940	-0.3296530683
C	1.5002137660	3.6757688905	1.6697853122
N	-0.1940750087	2.3071796432	0.7193099552
C	0.2508059817	3.1709655360	1.6760157509
C	0.6505677547	1.9113866862	-0.2833243888
C	2.3954644177	3.3137218927	0.6323486403
H	-0.4881943682	3.4178912229	2.4208119270
H	1.7979554646	4.3749582306	2.4379667429
C	2.8807969047	1.9293353377	-1.4406725933
H	2.8167969165	2.6069450936	-2.2976624921
H	3.9172092041	1.9476412038	-1.1040567345
C	2.4863098091	0.5303828878	-1.8906897034
H	3.0960750218	0.2196584434	-2.7392259387
H	2.6485400915	-0.1870771530	-1.0817488770
C	1.0257262419	0.5297593158	-2.2845211276
H	0.8737866159	1.1321076441	-3.1857097930
H	0.6677258132	-0.4778814631	-2.4943869151
N	0.2161525511	1.0585872726	-1.1998859406
H	-0.7556283196	0.7774582420	-1.0932330701
H	6.3976546103	4.5093297659	2.6606619499
C	5.7840029770	4.5394107361	1.7676119608
C	4.1852324487	4.6011161297	-0.5314822929
C	6.2203071870	5.1864700539	0.6202757059

C	4.5388205223	3.9264480405	1.7578098892
C	3.7379506541	3.9441901165	0.6144328622
C	5.4196227404	5.2152186819	-0.5228930805
H	4.1845593276	3.4155899926	2.6459471289
H	3.5576180676	4.6383233332	-1.4149296300
C	7.4608978859	5.9166192327	0.3266813974
C	9.5579136303	7.3639767663	-0.7372812184
C	8.5678438200	6.1791317363	1.1202549783
C	7.3980999107	6.3741771693	-0.9929390541
C	8.4463064732	7.0983849678	-1.5307000077
C	9.6176489910	6.9082521557	0.5764614681
H	8.6142268701	5.8239829123	2.1435936060
H	8.4067451336	7.4564672909	-2.5539842524
H	10.4909895199	7.1253088121	1.1801405862
H	10.3859339826	7.9314172447	-1.1457797067
C	6.0940976378	5.9632650655	-1.6567725795
C	6.3368800580	5.0358076266	-2.8550928923
H	6.8773958454	5.5640863754	-3.6432617688
H	5.3848360178	4.6934527624	-3.2674946036
H	6.9187489218	4.1596326329	-2.5627009299
C	5.2667368582	7.1776283637	-2.0950552940
H	5.7939278585	7.7383748491	-2.8696696452
H	5.0717957032	7.8458045295	-1.2542623176
H	4.3081365188	6.8529690813	-2.5063254185
C	-1.6632983098	1.8534524656	0.8628403395
O	-2.2187200457	2.3110208096	1.8488075823
O	-2.0718697643	1.1030995793	-0.0264264483

MA2 in gas phase

C	2.5325819074	-0.2268122514	-0.0740681710
C	4.4896027602	1.0621472825	-0.5427099790
C	4.7344576246	-0.9426253788	0.5212090268
N	5.2880059700	0.1580222611	0.0190028856
C	3.3595285211	-1.1814909207	0.5012424746
C	3.1019137861	0.9213245088	-0.6069992915
H	2.9502202722	-2.0823647785	0.9402240788
H	2.4945384022	1.6655197855	-1.1060365008
N	5.6067653745	-1.8684145234	1.0434449011
H	6.5303377552	-1.5199060616	1.2318779023
H	5.2426803406	-2.5235509363	1.7108872072
N	5.1196539559	2.1450554894	-1.1088131700
H	6.0755454768	2.2716977380	-0.8253983287
H	4.5837428187	2.9848190172	-1.2290481371
H	-1.1794687863	-2.8888639275	-0.8774253549

C	-0.8056356486	-1.9169229557	-0.5764940380
C	0.1782972503	0.5910071162	0.1728288235
C	-1.6747381622	-0.8845030595	-0.2650761567
C	0.5587312459	-1.6887767459	-0.5047715992
C	1.0658403269	-0.4424932962	-0.1338581486
C	-1.1829026641	0.3663227296	0.1113838720
H	1.2488905423	-2.4832034166	-0.7627471859
H	0.5694600747	1.5554514962	0.4791776531
C	-3.1417443202	-0.8355911832	-0.2448766176
C	-5.8237722749	-0.2022690130	-0.0404238181
C	-4.0904455432	-1.8059091839	-0.5327596466
C	-3.5308207035	0.4461784442	0.1461914938
C	-4.8716867294	0.7680086588	0.2487018247
C	-5.4350564633	-1.4793782718	-0.4273499443
H	-3.7942143943	-2.8040707717	-0.8347618737
H	-5.1857184300	1.7612469847	0.5515467288
H	-6.1896480259	-2.2254446785	-0.6472094526
H	-6.8778277600	0.0373841375	0.0365532397
C	-2.3231425495	1.3256137677	0.4180558388
C	-2.2968900970	1.7711582761	1.8845110370
H	-1.3934946577	2.3452061605	2.1001371086
H	-2.3229111563	0.9077478969	2.5513066941
H	-3.1604902359	2.4011172984	2.1094391281
C	-2.3060694117	2.5396471560	-0.5161139667
H	-1.4039933713	3.1350458418	-0.3612208120
H	-3.1704548614	3.1801922430	-0.3274346620
H	-2.3365985781	2.2249214119	-1.5604603608

MA2 in aqueous phase

C	-1.7862473064	0.9783575092	1.0115729059
C	0.2712046158	0.3525691350	-0.0418577506
C	0.3460688946	1.2383100878	2.0700774810
N	0.9918838437	0.7392253334	1.0132137800
C	-1.0426981544	1.3806052099	2.1146617426
C	-1.1212549282	0.4529433536	-0.0892712895
H	-1.5137435825	1.8152342525	2.9866767899
H	-1.6588650125	0.1036702578	-0.9613258999
N	1.1234514211	1.5778149643	3.1507778723
H	2.0970498253	1.7368422045	2.9485757291
H	0.7241604566	2.2232596024	3.8115941273
N	0.9704074017	-0.2081325593	-1.0835980333
H	1.9532373557	0.0100047845	-1.1093647909
H	0.5203971147	-0.2065435936	-1.9838290445
H	-5.9186431247	0.7314505834	3.1185172769
C	-5.3752393418	0.9371396794	2.2031917321

C	-3.9547488069	1.4378666148	-0.1575754389
C	-6.0435246805	1.2753879504	1.0365116089
C	-3.9913440937	0.8518758873	2.1804122104
C	-3.2670037481	1.0971765843	1.0109527030
C	-5.3330710290	1.5258644596	-0.1402816156
H	-3.4628866975	0.5680631040	3.0825157854
H	-3.4039003659	1.6422434420	-1.0695938661
C	-7.4773712599	1.4269077000	0.7544291564
C	-9.9973387774	1.8195515216	-0.3141132867
C	-8.5891240178	1.2799758471	1.5732018384
C	-7.6229521712	1.7677644841	-0.5921992625
C	-8.8818361735	1.9656460224	-1.1321834354
C	-9.8512496400	1.4790552190	1.0274238316
H	-8.4807708447	1.0127662142	2.6183186420
H	-9.0039752010	2.2292637574	-2.1775821060
H	-10.7311374773	1.3677862962	1.6505374715
H	-10.9892048090	1.9704194424	-0.7249232047
C	-6.2759904605	1.8620566258	-1.2866853909
C	-6.0340857868	3.2736137971	-1.8337959340
H	-5.0387177716	3.3479876055	-2.2765179695
H	-6.1196901083	4.0210310711	-1.0427743981
H	-6.7681865153	3.5077076699	-2.6081629118
C	-6.1705483089	0.8346249980	-2.4213280183
H	-5.1778030867	0.8654843138	-2.8749424309
H	-6.9059652162	1.0536527198	-3.1989020514
H	-6.3526334310	-0.1769111524	-2.0530335553

MA2-CO_2 in gas phase

C	1.5573958297	-0.1572073938	0.1673274494
C	3.5340084576	1.1369803377	-0.1990253144
C	3.7258186578	-0.8698730752	0.8818588563
N	4.3105328723	0.2177360691	0.3770156692
C	2.3531998662	-1.1056837426	0.7925195719
C	2.1503635489	0.9959675336	-0.3252911334
H	1.9199756341	-1.9966243197	1.2286303770
H	1.5647358268	1.7519004195	-0.8327104606
N	4.5457504364	-1.7529670631	1.5385998191
H	5.5282512854	-1.6597154034	1.3474292887
H	4.2132987765	-2.6936356392	1.6471500800
N	4.1691858522	2.2657328785	-0.6549284091
H	5.1638988394	2.1802619867	-0.7751210749
H	3.6958461789	2.8032950199	-1.3580653883
H	-2.0499289931	-2.8443418867	-0.9472974116
C	-1.7128881783	-1.8772931310	-0.5920991022

C	-0.8227029917	0.6197659137	0.3013983355
C	-2.6180760399	-0.8710890405	-0.2986322544
C	-0.3603419267	-1.6292835117	-0.4276665931
C	0.0998865968	-0.3880685111	0.0143944565
C	-2.1736104429	0.3730607628	0.1520489482
H	0.3597454157	-2.4030861234	-0.6657900264
H	-0.4680692617	1.5790216349	0.6634951372
C	-4.0843202692	-0.8492847670	-0.3631680123
C	-6.7856989904	-0.2743669542	-0.2906732167
C	-4.9940139959	-1.8227103655	-0.7494810629
C	-4.5215066304	0.4069399735	0.0584380647
C	-5.8725571494	0.6991162532	0.0967326828
C	-6.3488629588	-1.5253035235	-0.7103804452
H	-4.6598946869	-2.8005576699	-1.0772645139
H	-6.2243085053	1.6717406202	0.4239116439
H	-7.0735907738	-2.2735700637	-1.0090330505
H	-7.8472073753	-0.0577282630	-0.2653616937
C	-3.3494006284	1.2970519453	0.4327849906
C	-3.4119706519	1.6819059614	1.9154157595
H	-2.5347956174	2.2648312402	2.2030361472
H	-3.4544050855	0.7914393261	2.5446904743
H	-4.3003815616	2.2844181273	2.1177318175
C	-3.3088826313	2.5488849429	-0.4492911807
H	-2.4284918793	3.1539918232	-0.2235735257
H	-4.1947104267	3.1650425929	-0.2799277475
H	-3.2799815051	2.2771374728	-1.5056819417
C	7.0955136044	-0.1171810550	-0.6507279635
O	7.0303030446	0.8822206049	-1.2284809136
O	7.2176483470	-1.1248837805	-0.0965134245

MA2-CO_2 in aqueous phase

C	-1.7763863603	1.0416224848	1.0191577383
C	0.2610931666	0.3797972369	-0.0748184528
C	0.3498457594	1.3018126770	2.1131737195
N	0.9800803080	0.7736243730	1.0197555297
C	-1.0302517148	1.4473345719	2.1166018589
C	-1.1206332133	0.5050768781	-0.0792202992
H	-1.4936042078	1.8899473298	2.9870045720
H	-1.6604692723	0.1557399306	-0.9480405387
N	1.1045542277	1.7278731221	3.1458962273
H	2.0111025202	1.3035025458	3.2716454653
H	0.6117836609	2.0015251055	3.9787307532
N	0.9176778144	-0.1895046607	-1.1057341087
H	1.8903689495	0.0463342655	-1.2319196454
H	0.3804652963	-0.3651887591	-1.9375257611

H	-5.8959076128	0.8703474124	3.1470304229
C	-5.3551126079	1.0422793228	2.2235088047
C	-3.9424024009	1.4538742428	-0.1608943659
C	-6.0261869316	1.3296986252	1.0448293463
C	-3.9712640395	0.9640935623	2.2026043847
C	-3.2536105028	1.1631489368	1.0206615067
C	-5.3200113494	1.5378469339	-0.1432862958
H	-3.4415334412	0.7175135849	3.1146068464
H	-3.3957108605	1.6243786483	-1.0821043058
C	-7.4613108597	1.4591973649	0.7597571625
C	-9.9852301449	1.7883428027	-0.3181228243
C	-8.5700337632	1.3370636779	1.5868515186
C	-7.6115063009	1.7441961614	-0.5990351708
C	-8.8729680869	1.9098963244	-1.1441144617
C	-9.8343165271	1.5041934647	1.0361692032
H	-8.4571924362	1.1136346070	2.6416643466
H	-8.9992898587	2.1299376581	-2.1990020648
H	-10.7123418652	1.4121541487	1.6649327660
H	-10.9790193273	1.9148163210	-0.7325065670
C	-6.2670407079	1.8241453589	-1.2995036688
C	-6.0380974183	3.2181283369	-1.8957901587
H	-5.0437870129	3.2858718755	-2.3418000179
H	-6.1303988268	3.9919085053	-1.1313611625
H	-6.7750083961	3.4176463949	-2.6770668169
C	-6.1536402696	0.7584429223	-2.3973396218
H	-5.1629149410	0.7842825466	-2.8555872718
H	-6.8940557173	0.9422447918	-3.1792241239
H	-6.3234055081	-0.2413572446	-1.9929931123
C	2.5198292411	0.6139414460	1.0223510082
O	3.0588251737	1.0582386321	0.0161089904
O	2.9518923654	0.0679555331	2.0301376452

MA3 in gas phase

H	-1.9500436571	-2.2794591076	0.1645816117
C	-2.2868756322	-1.2638366266	0.0368069606
C	-1.9004980842	1.0815558959	-0.3076611335
N	-4.1262708839	0.2652941458	0.0105741185
C	-3.2712096871	1.2607325149	-0.1933744106
C	-3.6392405396	-0.9652581390	0.1177507240
C	-1.4036764907	-0.2124048495	-0.1836827103
H	-1.2608680886	1.9255621255	-0.5061616657
N	-4.6375231975	-1.9209419093	0.3364232554
N	-3.9090037757	2.5006191741	-0.2978935674
H	-4.9104663245	2.4275413155	-0.2288826519

H	-5.5556400839	-1.5144071302	0.4013483417
C	-3.3579025539	3.7518224602	-0.3938474914
C	-4.5301418286	-3.2854771525	0.4151112962
O	-2.1673212568	3.9627269410	-0.4493505889
O	-3.4839397147	-3.8876930032	0.3280789969
C	-4.3752036382	4.8703201180	-0.3921067676
H	-5.3122650333	4.5880778008	-0.8730173080
H	-3.9462166815	5.7308424371	-0.8990899594
H	-4.5888532970	5.1514838445	0.6412946946
C	-5.8503814587	-4.0008908031	0.5941787233
H	-5.6885178823	-4.8705659045	1.2271665507
H	-6.1895503703	-4.3533080686	-0.3817456962
H	-6.6278335456	-3.3713643380	1.0270403339
H	2.2543142744	-2.7634286559	-1.4773387098
C	1.8980094906	-1.8643880063	-0.9880841837
C	0.9557598862	0.4551964329	0.2550482997
C	2.7846392333	-0.9431933685	-0.4520860757
C	0.5373309024	-1.6207754521	-0.8929573203
C	0.0529007485	-0.4650286298	-0.2780330331
C	2.3098819768	0.2108392556	0.1701446727
H	-0.1641660710	-2.3292231759	-1.3176438568
H	0.5824803906	1.3450093861	0.7502046875
C	4.2502917637	-0.9293584929	-0.3918653613
C	6.9329195708	-0.4196774527	-0.0071042058
C	5.1826011252	-1.8382527268	-0.8661907404
C	4.6517698395	0.2318429178	0.2728144836
C	5.9951037206	0.4902900500	0.4677133778
C	6.5300095465	-1.5738455894	-0.6685985637
H	4.8683270588	-2.7387807187	-1.3817148489
H	6.3202406950	1.3875274950	0.9831098514
H	7.2740989939	-2.2722369241	-1.0323399126
H	7.9890634599	-0.2284749960	0.1397516461
C	3.4496251872	1.0617801105	0.6941960070
C	3.4512877111	2.4407367573	0.0261985960
H	3.4942432492	2.3442006521	-1.0597927332
H	4.3097559000	3.0302477640	0.3540160953
H	2.5440661645	2.9922983532	0.2824379512
C	3.3671000269	1.1979716107	2.2187273239
H	3.3488757959	0.2162907533	2.6949422960
H	2.4593102265	1.7329347183	2.5063592973
H	4.2237958368	1.7531516358	2.6057844713

MA3 in aqueous phase

H	0.8414680596	-0.2884198462	3.4904494986
C	0.9573737113	-0.7775081608	2.5376962706

C	1.2212018563	-0.7460982346	0.1504416755
N	1.0370000165	-2.8274772859	1.3068062173
C	1.1709106722	-2.1326981015	0.1825990793
C	0.9370724533	-2.1645457496	2.4547303396
C	1.1029654282	-0.0593062203	1.3546666253
H	1.3598009437	-0.2321837752	-0.7856685328
N	0.7960992626	-3.0183923653	3.5512641718
N	1.2616367195	-2.9455449919	-0.9509354499
H	1.2426389562	-3.9312493915	-0.7387791875
H	0.7859956759	-3.9938733101	3.2954029800
C	1.2993557655	-2.5930653198	-2.2691771835
C	0.7044961767	-2.7198707592	4.8787561295
O	1.3067771917	-1.4370504440	-2.6584535747
O	0.7044646515	-1.5805658861	5.3147775056
C	1.2968990440	-3.7563918699	-3.2260957879
H	1.6954660787	-4.6679537076	-2.7832568442
H	1.8740300612	-3.4885969350	-4.1088391388
H	0.2656027670	-3.9426998261	-3.5343466132
C	0.6346584243	-3.9221811653	5.7831820253
H	0.0003865479	-3.6871324875	6.6355771046
H	1.6413418174	-4.1302347125	6.1523453648
H	0.2615086437	-4.8106130307	5.2759289083
H	2.2166809401	4.0538440634	3.2224374035
C	1.7436388730	3.5209513113	2.4054216349
C	0.5476902943	2.1242109623	0.2950981655
C	1.1708595524	4.2040635507	1.3419077243
C	1.7124187861	2.1334712692	2.4060270813
C	1.1212422887	1.4236144206	1.3582552542
C	0.5755335597	3.5027110706	0.2919863680
H	2.1730744799	1.5905828377	3.2230952407
H	0.0707159615	1.5839020784	-0.5155756468
C	1.0525984796	5.6400354390	1.0568150381
C	0.5789916838	8.1646441623	0.0445268981
C	1.4808281478	6.7447782175	1.7778766072
C	0.3883181205	5.7916291789	-0.1642194776
C	0.1497708248	7.0541726168	-0.6758279563
C	1.2379314125	8.0109111643	1.2607873990
H	1.9953033994	6.6241731584	2.7246403915
H	-0.3624901419	7.1818970773	-1.6235763406
H	1.5644285745	8.8870936465	1.8084982444
H	0.3991056940	9.1596264491	-0.3455838400
C	0.0202566115	4.4428113450	-0.7609511490
C	0.7002634329	4.2154077322	-2.1173637197
H	1.7843434511	4.3146536994	-2.0357902623
H	0.3394998310	4.9390676691	-2.8512114980

H	0.4741130978	3.2136662701	-2.4900318312
C	-1.4979807068	4.2785627500	-0.9054362296
H	-2.0020229993	4.4213370329	0.0522120247
H	-1.7358047017	3.2777726445	-1.2734560809
H	-1.8942903446	5.0043122591	-1.6185895370

MA3-CO_2 in gas phase

H	-1.1603909129	-2.3865536854	0.1229635745
C	-1.5362375794	-1.3834810446	0.0066332631
C	-1.2441052938	0.9777201514	-0.3036831462
C	-2.6213381253	1.1021140716	-0.1938023208
C	-2.9000912931	-1.1443438326	0.0867610686
C	-0.6950127700	-0.2959762047	-0.1972607893
H	-0.6399108516	1.8506604601	-0.4878326422
N	-3.8481395882	-2.1506826385	0.2894003063
N	-3.2979411278	2.3206455111	-0.2854255623
H	-4.2987819086	2.2254341903	-0.2337191828
H	-4.7898218729	-1.8039257846	0.3652377241
C	-2.7867031793	3.5885278264	-0.3834715905
C	-3.6730930621	-3.5100758915	0.3399556829
O	-1.6038164563	3.8415811726	-0.4342674571
O	-2.5998914235	-4.0612281856	0.2424696004
C	-3.8382225881	4.6746424047	-0.3941254822
H	-4.8231162557	4.3176383068	-0.6951421973
H	-3.5115913838	5.4664760780	-1.0647665924
H	-3.9117776927	5.0941316794	0.6109924543
C	-4.9593632254	-4.2882396640	0.5025090564
H	-4.7626554647	-5.1540764016	1.1310873596
H	-5.2711038626	-4.6493291079	-0.4793705877
H	-5.7701905542	-3.6978439599	0.9290929362
H	3.0480740555	-2.7070606281	-1.5082959463
C	2.6615168963	-1.8250502072	-1.0110012697
C	1.6404619036	0.4498077800	0.2530321213
C	3.5160209891	-0.8828051238	-0.4597415387
C	1.2936761216	-1.6261348361	-0.9186866745
C	0.7697378029	-0.4936605121	-0.2925718116
C	3.0021837676	0.2489631628	0.1723278992
H	0.6170053548	-2.3522050374	-1.3537656837
H	1.2370976153	1.3218366127	0.7563178199
C	4.9798964467	-0.8259919784	-0.3888814830
C	7.6430954511	-0.2450331861	0.0265545858
C	5.9417554824	-1.7024593032	-0.8651846957
C	5.3419155533	0.3383755981	0.2924964859
C	6.6755972585	0.6325507611	0.5028006182

C	7.2791942205	-1.4022398832	-0.6521404994
H	5.6577411336	-2.6056006743	-1.3936217452
H	6.9704897226	1.5322992615	1.0319015006
H	8.0461162902	-2.0750811051	-1.0167379003
H	8.6920421526	-0.0260005319	0.1858260150
C	4.1125373607	1.1281187162	0.7133643019
C	4.0774997710	2.5133395474	0.0594085726
H	4.1301593827	2.4294730191	-1.0272436882
H	4.9162843379	3.1242605853	0.3989296543
H	3.1528170407	3.0353308942	0.3152999708
C	4.0153854051	1.2462315435	2.2385189651
H	3.0898715623	1.7506935736	2.5249329758
H	4.8522078269	1.8231548404	2.6371991514
H	4.0237063860	0.2596509396	2.7048685870
N	-3.4399337853	0.0684854822	-0.0071491139
C	-6.5272736803	0.4373671047	0.1037957675
O	-6.4080106830	1.5702162413	-0.0932648297
O	-6.6890779865	-0.6900822298	0.3028657505

MA3-CO_2 in aqueous phase

H	3.2078448947	4.8683794905	5.3235785319
C	3.2658475017	4.4056738893	4.3524702531
C	3.4825036652	4.4998708574	1.9722603313
C	3.3007696233	3.1357367306	1.9139828718
C	3.1083145774	3.0376539608	4.2617782484
C	3.4533473245	5.1554365846	3.1973198060
H	3.6649340539	5.0312780645	1.0540674454
N	2.9063138078	2.2298172507	5.3607790687
N	3.3123682798	2.4300140967	0.7287007628
H	3.5708888270	1.4534632849	0.8065126104
H	2.4082040376	1.3666358012	5.1780183821
C	2.9847042412	2.9104419428	-0.5224049364
C	3.3486565524	2.4586310121	6.6465343944
O	2.6083450061	4.0467634506	-0.7212197866
O	4.0078003816	3.4282739753	6.9587218715
C	3.1136506973	1.8774392932	-1.6059902072
H	4.1035947844	1.4198611715	-1.5823396536
H	2.9434272523	2.3463887160	-2.5711962210
H	2.3750552761	1.0887777801	-1.4484399870
C	2.9379336841	1.3825871838	7.6114128328
H	3.3695860659	1.5882889086	8.5868537205
H	3.2736891211	0.4074558966	7.2545862779
H	1.8493804658	1.3540430887	7.6885315231
H	4.9226199291	9.0921738559	5.1825144860
C	4.4155128136	8.6243006529	4.3466597295

C	3.1301942795	7.3958370279	2.1834104625
C	3.9391285644	9.3805382980	3.2843228211
C	4.2439390955	7.2479975259	4.3204216806
C	3.6099428985	6.6233161478	3.2437459806
C	3.2950403667	8.7627889908	2.2102423619
H	4.6318978762	6.6474776943	5.1348279326
H	2.6173091812	6.9230845038	1.3529229342
C	3.9795275136	10.8245792049	3.0208593572
C	3.8015762612	13.3978279593	2.0396140810
C	4.5160505075	11.8655842986	3.7642475244
C	3.3567275139	11.0635866454	1.7921091057
C	3.2645507391	12.3514743843	1.2966652210
C	4.4219184185	13.1569124214	3.2622665076
H	5.0008841624	11.6765726241	4.7153789097
H	2.7846132905	12.5467937674	0.3436014910
H	4.8362820890	13.9844527094	3.8258000926
H	3.7376108788	14.4116890875	1.6621561865
C	2.8605320102	9.7711024662	1.1649920501
C	3.5417815023	9.4952441500	-0.1820104368
H	4.6282180359	9.4769927762	-0.0771248270
H	3.2759625436	10.2654831956	-0.9087609309
H	3.2184313725	8.5297664890	-0.5780428567
C	1.3368820894	9.7678170132	0.9905408240
H	1.0037407671	8.8039085663	0.5989222061
H	1.0327631460	10.5432495703	0.2846023276
H	0.8318370714	9.9458376241	1.9416681583
N	3.1182534209	2.4163121662	3.0521010907
C	2.9084967143	0.8392269321	2.9640157833
O	3.7866793862	0.2904992253	2.3225020230
O	1.9069666993	0.4722625796	3.5522153681

B. Dimer-receptors

Dimer in gas phase

H	5.4693137757	-2.7754289207	-0.9322627486
C	5.8106815511	-1.8183138299	-0.5549037601
C	6.7036782488	0.6529722519	0.4171247473
C	4.9076498881	-0.8155993982	-0.2363581045
C	7.1663949511	-1.5766652099	-0.3836177325
C	7.6104867467	-0.3512272172	0.0985168369
C	5.3522874166	0.4163917223	0.2480512388
H	7.8855730789	-2.3494648646	-0.6277340209
H	7.0601614274	1.6064144525	0.7921812779
C	3.4416236398	-0.7784280552	-0.3150906193

C	0.7243205631	-0.1604510740	-0.2795619032
C	2.5219192581	-1.7278494824	-0.7317413755
C	3.0085446134	0.4743903825	0.1206324794
C	1.6634294343	0.7836917313	0.1414887373
C	1.1729672521	-1.4106361343	-0.7116385665
H	2.8441406114	-2.7021453294	-1.0812139759
H	1.3238438535	1.7501773457	0.4991484239
H	0.4495504125	-2.1367778375	-1.0637831013
C	4.1845026949	1.3491452174	0.5226622698
H	-2.8441406114	2.7021453294	-1.0812139759
C	-2.5219192581	1.7278494824	-0.7317413755
C	-1.6634294343	-0.7836917313	0.1414887373
C	-3.4416236398	0.7784280552	-0.3150906193
C	-1.1729672521	1.4106361343	-0.7116385665
C	-0.7243205631	0.1604510740	-0.2795619032
C	-3.0085446134	-0.4743903825	0.1206324794
H	-0.4495504125	2.1367778375	-1.0637831013
H	-1.3238438535	-1.7501773457	0.4991484239
C	-4.9076498881	0.8155993982	-0.2363581045
C	-7.6104867467	0.3512272172	0.0985168369
C	-5.8106815511	1.8183138299	-0.5549037601
C	-5.3522874166	-0.4163917223	0.2480512388
C	-6.7036782488	-0.6529722519	0.4171247473
C	-7.1663949511	1.5766652099	-0.3836177325
H	-5.4693137757	2.7754289207	-0.9322627486
H	-7.0601614274	-1.6064144525	0.7921812779
H	-7.8855730789	2.3494648646	-0.6277340209
H	-8.6723929715	0.1782141386	0.2264064859
C	-4.1845026949	-1.3491452174	0.5226622698
C	4.2593736219	2.6068205629	-0.3508625951
H	5.1460400433	3.1953358753	-0.1051417274
H	3.3818686812	3.2376219955	-0.1928688820
H	4.3059034048	2.3430355512	-1.4085669528
C	4.1149386230	1.7305573952	2.0054533779
H	4.9973576224	2.3042276685	2.2971607188
H	4.0625796687	0.8400949558	2.6336696990
H	3.2332320605	2.3433306972	2.2052956738
C	-4.1149386230	-1.7305573952	2.0054533779
H	-3.2332320605	-2.3433306972	2.2052956738
H	-4.9973576224	-2.3042276685	2.2971607188
H	-4.0625796687	-0.8400949558	2.6336696990
C	-4.2593736219	-2.6068205629	-0.3508625951
H	-3.3818686812	-3.2376219955	-0.1928688820
H	-4.3059034048	-2.3430355512	-1.4085669528
H	-5.1460400433	-3.1953358753	-0.1051417274

H	8.6723929715	-0.1782141386	0.2264064859

Dimer in aqueous phase

H	-0.0529052572	3.4181807512	2.5351185560
C	0.4141994730	2.4709418615	2.7808742183
C	1.6179504246	0.0173450656	3.4236697641
C	0.6858430559	1.5337751297	1.7942830242
C	0.7484597217	2.1707105183	4.0958087817
C	1.3456718458	0.9551381507	4.4151603514
C	1.2854861190	0.3108021137	2.1136878834
H	0.5413022287	2.8889993407	4.8803416169
H	2.0818481593	-0.9294796235	3.6796025885
C	0.4398690703	1.5610320944	0.3445416823
C	0.1906811745	1.0515999524	-2.3890879520
C	-0.1316256180	2.5205479914	-0.4801451352
C	0.8907776821	0.3559153992	-0.1954917386
C	0.7723571611	0.1006842694	-1.5465477966
C	-0.2515322890	2.2582351351	-1.8385770487
H	-0.4947365917	3.4592045861	-0.0771985569
H	1.1387009471	-0.8330764822	-1.9602502639
H	-0.7186927829	2.9949802847	-2.4823010319
C	1.4712090466	-0.5502086406	0.8736354336
H	-0.7139194412	-1.8531079328	-5.8923393975
C	-0.4419681070	-0.8467338816	-5.5942767515
C	0.2442530411	1.7511248298	-4.8039278471
C	-0.2214704577	0.1427439178	-6.5392796386
C	-0.3115530222	-0.5286045325	-4.2520786040
C	0.0366530962	0.7612205882	-3.8375396938
C	0.1167567446	1.4390593248	-6.1447963550
H	-0.4954012004	-1.2948135132	-3.5081379223
H	0.5285341514	2.7528342783	-4.4989154048
C	-0.2643907586	0.0952363849	-8.0058958242
C	-0.1867350783	0.5540042525	-10.7298437006
C	-0.5391428051	-0.9522619952	-8.8751109882
C	0.0487995011	1.3659235319	-8.4924634175
C	0.0880918192	1.6013476765	-9.8559697591
C	-0.4974146878	-0.7122678396	-10.2428316459
H	-0.7794697834	-1.9409584249	-8.4999792689
H	0.3309571575	2.5846914877	-10.2447224143
H	-0.7065760700	-1.5175015577	-10.9378213314
H	-0.1574993308	0.7242486144	-11.8000932298
C	0.3166895179	2.3376934248	-7.3566660431
C	0.6802503743	-1.8618907616	0.9671145088
H	1.0638481242	-2.4843239091	1.7781730374
H	0.7726492045	-2.4246694999	0.0352668069

H	-0.3792483277	-1.6703871454	1.1479320457
C	2.9499249629	-0.8516386639	0.6014992805
H	3.3722061614	-1.4548598638	1.4078285433
H	3.5294841367	0.0694766195	0.5163980451
H	3.0549975595	-1.4112263735	-0.3309256383
C	1.7494618256	2.8781580985	-7.4272386503
H	1.9585713053	3.5248217610	-6.5728197277
H	1.8888280920	3.4621291989	-8.3396638979
H	2.4733689661	2.0606344278	-7.4292983674
C	-0.6924954676	3.4914722678	-7.3744788325
H	-0.5355487027	4.1515053614	-6.5191415550
H	-1.7160015936	3.1126959874	-7.3376843378
H	-0.5771746539	4.0803716887	-8.2870632326
H	1.5985764164	0.7354385150	5.4458311860

DA1 in gas phase

C	7.1194728901	-0.3770345018	-0.1166314046
C	7.0213585213	1.7848550284	0.9232755730
N	9.1081982270	0.9790943680	0.0872138077
C	8.3747660440	1.9086001805	0.6893398307
C	8.4950216554	-0.1328597601	-0.3107438203
C	6.3828634428	0.6140999111	0.5109256230
H	8.9075159364	2.8022458264	1.0005476476
H	6.4659774917	2.5713113736	1.4170575752
C	6.5134845719	-1.6846919994	-0.5706943826
H	6.4043949716	-2.3511793767	0.2922810149
H	5.5025335148	-1.5174246628	-0.9465703059
C	7.3674106260	-2.3671977021	-1.6340089578
H	7.0087846730	-3.3821684033	-1.8152903688
H	7.2954423766	-1.8193096379	-2.5775202005
C	8.8239763448	-2.4002296428	-1.1990736938
H	8.9242756388	-3.0281653024	-0.3014838630
H	9.4469347505	-2.8440025215	-1.9777768602
N	9.2786290579	-1.0500139013	-0.9618988644
H	10.2648497295	-0.8705041806	-0.8891449392
H	2.7662287807	-0.7182568263	3.1091274610
C	3.1055456218	-0.2850294037	2.1752173211
C	4.0036531795	0.8370217218	-0.2241564334
C	2.2013826485	0.1128114393	1.2041386374
C	4.4626994195	-0.1182152727	1.9380785993
C	4.9217362708	0.4408881362	0.7477766218
C	2.6524924186	0.6708424044	0.0052847424
H	5.1834790465	-0.4255464586	2.6867792962
H	4.3643931379	1.2696381283	-1.1519071534
C	0.7332090497	0.0708425724	1.1708334393

C	-1.9863315420	0.2667655497	0.5816899970
C	-0.1995299792	-0.3932343224	2.0861714260
C	0.3083687118	0.6152498836	-0.0413729578
C	-1.0355830602	0.7185060707	-0.3348511136
C	-1.5496552545	-0.2946532114	1.7830068146
H	0.1108504202	-0.8202597848	3.0327517076
H	-1.3660444677	1.1298841917	-1.2831761775
H	-2.2858576904	-0.6334582677	2.5030380520
C	1.4869257953	1.0150707241	-0.9097893062
C	1.4472127960	2.5052318235	-1.2598278129
H	0.5643535872	2.7325758944	-1.8620114266
H	2.3281637739	2.7923307207	-1.8376101238
H	1.4115492740	3.1184936628	-0.3584041617
C	1.5181780898	0.1707238378	-2.1916001605
H	0.6359330163	0.3728813621	-2.8034105673
H	1.5309385682	-0.8947698188	-1.9568090109
H	2.4027536095	0.4036148428	-2.7882484018
H	-5.6362810144	2.7141379240	-0.8994170549
C	-5.2734887066	1.7668265964	-0.5173035937
C	-4.3167626904	-0.6589493688	0.4921477825
C	-6.1378245370	0.7059109621	-0.3031844759
C	-3.9288351698	1.6043540682	-0.2268461839
C	-3.4327387816	0.4014775459	0.2805478312
C	-5.6570313684	-0.5059838394	0.1965666719
H	-3.2474703511	2.4342048592	-0.3726433644
H	-3.9368194936	-1.6050174926	0.8643205065
C	-7.5844399497	0.5805430351	-0.5181774813
C	-10.2305350855	-0.1903345111	-0.7301857750
C	-8.5190869000	1.4898883699	-0.9906147690
C	-7.9703417809	-0.7105180648	-0.1540724315
C	-9.2926224924	-1.1006457103	-0.2580722086
C	-9.8454660140	1.0945345419	-1.0935635065
H	-8.2257511872	2.4934415965	-1.2761218424
H	-9.6024808374	-2.1020053969	0.0218072440
H	-10.5886278460	1.7922403154	-1.4609685955
C	-6.7800798474	-1.5270250895	0.3192056471
C	-6.9698978812	-2.0009183964	1.7637077751
H	-7.8229537949	-2.6798530268	1.8343678248
H	-7.1504629768	-1.1578922419	2.4321016413
H	-6.0859480167	-2.5372421413	2.1154238454
C	-6.5460060151	-2.7289389138	-0.6052419536
H	-7.3953165524	-3.4149772120	-0.5624459807
H	-5.6524378955	-3.2812323462	-0.3068557987
H	-6.4218877955	-2.4071925005	-1.6402723404
H	-11.2701511356	-0.4839643396	-0.8161947177

DA1 in aqueous phase

C	2.7489181581	4.3896328909	2.7672395089
C	2.9233002209	3.7927517932	0.4432164335
N	0.8696006733	3.4031170000	1.5966028385
C	1.6224771216	3.3510978841	0.4980713648
C	1.4138974289	3.9183924704	2.7025134069
C	3.5038724195	4.3172208055	1.6069744192
H	1.1492193139	2.9275178931	-0.3834476737
H	3.4927243155	3.7192201023	-0.4742974085
C	3.2588967632	4.9720058110	4.0643800189
H	3.8125315429	4.2082812403	4.6200292306
H	3.9689441022	5.7736498063	3.8537003292
C	2.1168178972	5.4858460528	4.9337886350
H	2.4925151631	5.7841321649	5.9134238986
H	1.6616395210	6.3664201628	4.4709386718
C	1.0598886935	4.4074265064	5.0940937936
H	1.4787763754	3.5579230504	5.6491605977
H	0.2052008430	4.7804691096	5.6595770092
N	0.5941017224	4.0000707104	3.7862309293
H	-0.2887789026	3.5255210661	3.7061859963
H	7.9618618820	4.1671709769	2.9379765549
C	7.2183411092	4.6120133149	2.2863014044
C	5.2881870909	5.7272311131	0.5918475893
C	7.5742396245	5.5597204221	1.3375600194
C	5.8880879594	4.2297177786	2.3833904999
C	4.9167640628	4.7766179353	1.5435216654
C	6.6095868246	6.1168353771	0.4968966127
H	5.5982553099	3.4782527078	3.1085543191
H	4.5355673764	6.1506641979	-0.0657348043
C	8.8756514676	6.1378364695	0.9866721714
C	11.0469617569	7.5139364025	-0.0803448117
C	10.1426733231	5.9016774212	1.4957731506
C	8.6882436427	7.0488753481	-0.0556309770
C	9.7615016547	7.7382710327	-0.5835208117
C	11.2179058631	6.5886918349	0.9544398338
H	10.2976818233	5.1828151725	2.2924009073
H	9.6092185485	8.4605160481	-1.3786275239
H	12.2144800691	6.3893647921	1.3299211081
C	7.2256051134	7.1111709810	-0.4705874681
C	7.0374354013	6.6480131961	-1.9219540772
H	7.5383659177	7.3324058233	-2.6097828225
H	5.9755499268	6.6268589108	-2.1776304811
H	7.4459708219	5.6465356225	-2.0708128017
C	6.6298362629	8.5111538489	-0.2869444489
H	7.1249394920	9.2268300938	-0.9465066016

H	6.7406365252	8.8533850910	0.7435792303
H	5.5658355115	8.5028147691	-0.5343635663
H	13.4103391721	9.4282741136	-3.5994756411
C	13.3773432069	9.2062830088	-2.5386677757
C	13.2767690006	8.6112158192	0.1925843322
C	14.4219019216	9.5677971762	-1.7003464279
C	12.2854418462	8.5408224948	-2.0012842878
C	12.2174698810	8.2350953465	-0.6382762740
C	14.3688201770	9.2665275408	-0.3392855466
H	11.4771324250	8.2356219520	-2.6560735877
H	13.2303782252	8.3985056318	1.2552040433
C	15.6861876423	10.2624847226	-1.9706287529
C	18.1526515334	11.4996116086	-1.9292991985
C	16.2046682555	10.7679072581	-3.1540441917
C	16.3917440123	10.3729279629	-0.7691489974
C	17.6287153904	10.9913428592	-0.7439685073
C	17.4464385903	11.3894618057	-3.1234785330
H	15.6538821875	10.6816731567	-4.0843908616
H	18.1865071787	11.0813654586	0.1820775301
H	17.8692096385	11.7916387821	-4.0368709284
C	15.6156514933	9.7472695141	0.3783790953
C	16.3769741554	8.5686102567	0.9954576279
H	17.3085951580	8.9099407944	1.4509158717
H	16.6157277518	7.8216485828	0.2354376094
H	15.7721560846	8.0901868141	1.7688207593
C	15.2675960550	10.7847386860	1.4514376684
H	16.1754146786	11.1720054587	1.9181561079
H	14.6486920543	10.3326046257	2.2295252588
H	14.7166415671	11.6213806252	1.0168468503
H	19.1206779827	11.9868897418	-1.9231751132

DA1-CO_2 in gas phase

C	6.2683042220	-0.7075740591	0.2977517077
C	6.0947776936	1.4780404800	-0.6840255160
N	8.2281239814	0.6800514701	0.0271804974
C	7.4525925881	1.6196520091	-0.5059551821
C	7.6533778848	-0.4556791275	0.4225466857
C	5.4924211203	0.2811667055	-0.2836736045
H	7.9608721849	2.5280606917	-0.8145931433
H	5.5078197420	2.2631584120	-1.1418617471
C	5.7128593239	-2.0114132240	0.8190734493
H	5.3509481374	-1.8654459216	1.8434388140
H	4.8441453243	-2.3162075961	0.2361904234
C	6.7712689112	-3.1081310741	0.8080138733

H	6.3897862949	-4.0124520275	1.2856457605
H	7.0264743801	-3.3642826233	-0.2242722998
C	8.0234903736	-2.6356377820	1.5282948518
H	7.8060810358	-2.5149822552	2.5987470056
H	8.8182214977	-3.3791763121	1.4417624046
N	8.4871856792	-1.4001616203	0.9434554808
H	9.4428294386	-1.1145872146	1.0656161995
H	1.8982776283	-1.6584733456	-2.4925470795
C	2.2287400291	-0.9749007799	-1.7189243361
C	3.1030753359	0.8004180681	0.2588671799
C	1.3146395472	-0.2722161440	-0.9501542331
C	3.5817941855	-0.7866535169	-1.4883458650
C	4.0311913015	0.0911981039	-0.5017861991
C	1.7516704118	0.6160726410	0.0336083654
H	4.3099451800	-1.3231104492	-2.0862871149
H	3.4544918953	1.4862197520	1.0228017624
C	-0.1530483853	-0.2652970793	-0.9652941103
C	-2.8812127207	0.1524434311	-0.5677408335
C	-1.0700903214	-0.9617830154	-1.7381021100
C	-0.5957409683	0.6327694233	0.0051220712
C	-1.9449443611	0.8422108019	0.2052610312
C	-2.4245221845	-0.7478681084	-1.5327477438
H	-0.7436336516	-1.6587974890	-2.5015965123
H	-2.2910560873	1.5249557043	0.9742110310
H	-3.1468550147	-1.2698027105	-2.1501039407
C	0.5715859884	1.2741770975	0.7327639318
C	0.5390975621	0.9313167276	2.2257569116
H	-0.3528385560	1.3516592605	2.6956424467
H	1.4141613937	1.3375007827	2.7368433175
H	0.5235124290	-0.1496341596	2.3740323665
C	0.5720778113	2.7925302252	0.5247522795
H	-0.3195241295	3.2396010658	0.9701876449
H	0.5798106128	3.0372081476	-0.5386652044
H	1.4477706660	3.2492253150	0.9900304373
C	10.9915491021	1.1341491137	-0.1525598800
O	10.8034097656	2.1155595024	-0.7312990748
O	11.2616974697	0.1638731250	0.4214523745
H	-6.5157747754	2.9369924712	0.1909254445
C	-6.1638304973	1.9218976257	0.0469103855
C	-5.2344910912	-0.6848323039	-0.3509179864
C	-7.0438846605	0.8525728049	0.0664389366
C	-4.8172850112	1.6773976411	-0.1680546456
C	-4.3326063795	0.3819787877	-0.3628778024
C	-6.5778295112	-0.4477511832	-0.1371228911
H	-4.1247526234	2.5097625778	-0.2064597043

H	-4.8671314944	-1.6973918836	-0.4834710542
C	-8.4955456473	0.7991315755	0.2804881470
C	-11.1560772358	0.1296377862	0.6248650721
C	-9.4213787938	1.8033003898	0.5218950978
C	-8.8985908861	-0.5353836129	0.2087431349
C	-10.2275857379	-0.8751117144	0.3812066677
C	-10.7548742215	1.4584222213	0.6931841242
H	-9.1156081124	2.8416671672	0.5766767662
H	-10.5503605496	-1.9096105957	0.3282248877
H	-11.4910858107	2.2307353170	0.8817775552
C	-7.7210755766	-1.4514286920	-0.0762816883
C	-7.9054379937	-2.1712648403	-1.4187668805
H	-8.7734179458	-2.8337836340	-1.3811635945
H	-7.0295164807	-2.7787471342	-1.6564715219
H	-8.0588093587	-1.4560639540	-2.2281172411
C	-7.5272234864	-2.4758044534	1.0469070564
H	-8.3924333130	-3.1398737176	1.1105081184
H	-7.4054664643	-1.9821582452	2.0119889656
H	-6.6452586287	-3.0923575444	0.8610811340
H	-12.2007040197	-0.1239638213	0.7620823297

DA1-CO_2 in aqueous phase

C	-1.9693822589	-1.6924329785	0.2159371027
C	-2.9494113030	-0.1498026699	1.7833697078
N	-4.2688866825	-1.9354794089	0.9366078683
C	-4.1094870567	-0.8331742045	1.7228411290
C	-3.2205918100	-2.3873148371	0.1804766337
C	-1.8463019894	-0.5758990616	1.0029132775
H	-4.9914891711	-0.5586150344	2.2783107872
H	-2.8794549094	0.7306975446	2.4060069503
C	-0.8394069822	-2.2602717235	-0.6080833505
H	-0.8326832558	-1.7929548741	-1.5977282433
H	0.1107975560	-2.0095057412	-0.1369578234
C	-0.9749346849	-3.7670051838	-0.7727967010
H	-0.1910948033	-4.1486687720	-1.4271850615
H	-0.8713343263	-4.2622467907	0.1965295671
C	-2.3304867910	-4.0845151972	-1.3641665963
H	-2.3901952132	-3.7262705641	-2.3966155641
H	-2.5207478799	-5.1576181991	-1.3733799279
N	-3.3801338987	-3.4669891401	-0.5710247014
H	-4.3181921835	-3.8599047893	-0.5580033722
H	1.6391801418	1.4170071798	3.3246985702
C	1.1749610399	1.2293453208	2.3633187800
C	-0.0313746712	0.7238399026	-0.1149033060
C	1.7338948504	1.7168809500	1.1909304362

C	0.0046958432	0.4878187721	2.2875020306
C	-0.5958758729	0.2194823990	1.0565312067
C	1.1266912371	1.4695416274	-0.0419268314
H	-0.4429699023	0.0950493457	3.1933920331
H	-0.5084643293	0.5357280892	-1.0706596211
C	2.9483449949	2.5035782868	0.9510777644
C	5.1236428483	3.9106907082	-0.0573211077
C	3.9055645091	2.9870584656	1.8290597656
C	3.0644119402	2.7295747142	-0.4225188661
C	4.1411169060	3.4317095693	-0.9279100406
C	4.9873112077	3.6851557270	1.3159614454
H	3.8154083390	2.8238949117	2.8969126308
H	4.2435512631	3.5877107626	-1.9969764106
H	5.7386230697	4.0742894725	1.9930823597
C	1.9095411263	2.0946284129	-1.1823138275
C	2.3971180249	1.0244657527	-2.1674946377
H	3.0109097985	1.4763686223	-2.9494942065
H	1.5454411068	0.5355295859	-2.6462423061
H	2.9892493028	0.2614272567	-1.6588607904
C	1.0726026141	3.1437821666	-1.9253486148
H	1.6719435908	3.6316594661	-2.6968896257
H	0.6993162067	3.9078744106	-1.2410351370
H	0.2169757440	2.6693630394	-2.4114830550
C	-5.6672008066	-2.5890611790	0.9825460320
O	-6.4135276731	-2.0817906925	1.8045525108
O	-5.8390781274	-3.5181529009	0.1901661079
H	7.2093896665	7.0033339775	-2.8449143390
C	7.3192618971	6.2550943133	-2.0678468156
C	7.5780804436	4.3318636878	-0.0535071514
C	8.5658916710	5.9533054111	-1.5379122221
C	6.2037263261	5.5843807532	-1.5855202344
C	6.3159750158	4.6249142862	-0.5753299737
C	8.6905463021	4.9891076111	-0.5372217876
H	5.2243669117	5.8201759836	-1.9871321493
H	7.6785023981	3.5704315107	0.7128169464
C	9.9050059195	6.4713652954	-1.8452995572
C	12.5935409338	7.0725217546	-2.0343622508
C	10.3172159436	7.4322439897	-2.7569912287
C	10.8292676242	5.8086028403	-1.0320210522
C	12.1765194649	6.1069146724	-1.1227549780
C	11.6716724614	7.7279718220	-2.8450834240
H	9.5990800269	7.9414544927	-3.3904058214
H	12.9015843723	5.5971538283	-0.4971979012
H	12.0142512124	8.4745081730	-3.5521486361
C	10.1396651665	4.7913508064	-0.1375634197

C	10.3521086315	5.0958882665	1.3484952887
H	11.4080225599	5.0072569924	1.6114371702
H	9.7873932227	4.3910731807	1.9629273619
H	10.0170799741	6.1065590438	1.5898631322
C	10.5965985469	3.3629176366	-0.4617941505
H	11.6587026444	3.2400432780	-0.2409742194
H	10.4325781101	3.1321005653	-1.5164922070
H	10.0369748868	2.6414733707	0.1377975440
H	13.6466309875	7.3149439369	-2.1160888952

DA2 in gas phase

C	-6.6949455226	-0.2341922062	0.1200160608
C	-8.9780165686	-0.6674485460	-0.4432352152
C	-8.5335370512	0.7551087056	1.2854474801
N	-9.4262799785	0.1426445763	0.5122008533
C	-7.1548657567	0.6024144625	1.1284767226
C	-7.6206073747	-0.8854928179	-0.6837484607
H	-6.4675420870	1.0902751417	1.8073909033
H	-7.3031795826	-1.5306995582	-1.4927795848
H	-3.0126994630	-2.9218766028	-0.7497338868
C	-3.3826463644	-1.9235989157	-0.5458505681
C	-4.3553288493	0.6366508766	0.0120782244
C	-2.5143672925	-0.8488337036	-0.4381181145
C	-4.7399170184	-1.7088368310	-0.3701383812
C	-5.2410884264	-0.4372074999	-0.0869567230
C	-3.0026019867	0.4274813049	-0.1619631421
H	-5.4270552431	-2.5451743416	-0.4239160900
H	-4.7443101937	1.6295037497	0.2116050422
C	-1.0557585430	-0.7729058858	-0.5399075001
C	1.6406634105	-0.1016765781	-0.5321582188
C	-0.1133354975	-1.7595474209	-0.7742795111
C	-0.6628513608	0.5492476842	-0.3248762032
C	0.6759423449	0.8866084986	-0.3210487972
C	1.2269304186	-1.4147363828	-0.7696751200
H	-0.4132832216	-2.7854710349	-0.9560456242
H	0.9894280964	1.9053796713	-0.1182592321
H	1.9734121488	-2.1754894525	-0.9648359333
C	-1.8741833292	1.4398847818	-0.0873860255
C	-2.0204046105	2.4913121580	-1.1931568963
H	-2.9346013159	3.0718145172	-1.0500851333
H	-2.0708500222	2.0155377433	-2.1739547688
H	-1.1745042664	3.1816190180	-1.1875599284
C	-1.8268540388	2.1046935380	1.2913139913
H	-2.7386790269	2.6790351828	1.4703264817

H	-0.9779875986	2.7871192011	1.3658885730
H	-1.7366157581	1.3549941123	2.0790207639
H	5.3472154118	2.5471496651	-1.4908909423
C	4.9656154503	1.6492136381	-1.0183891114
C	3.9577728931	-0.6661258082	0.1714348197
C	5.8183254649	0.7616913538	-0.3794923490
C	3.6080543946	1.3671438164	-1.0621523609
C	3.0874538771	0.2119110642	-0.4764673162
C	5.3075821409	-0.3921446918	0.2144191224
H	2.9378534064	2.0401828271	-1.5847666040
H	3.5584015135	-1.5529281166	0.6522703601
C	7.2732967355	0.7714450812	-0.1853620915
C	9.9206100227	0.2910150533	0.4346219734
C	8.2372242351	1.6781761370	-0.5957871090
C	7.6288668558	-0.3744734271	0.5314593635
C	8.9519796289	-0.6178317264	0.8449749763
C	9.5654445611	1.4283275245	-0.2806467116
H	7.9626581224	2.5642862453	-1.1566130143
H	9.2380213010	-1.5046826094	1.4003536208
H	10.3329161040	2.1246707939	-0.5963891797
C	6.4064801085	-1.2199175674	0.8527754648
C	6.1874337609	-1.3555104645	2.3636584740
H	5.2677040755	-1.9084723522	2.5685494462
H	6.1069182494	-0.3754521634	2.8358908247
H	7.0146618305	-1.8957201230	2.8288021220
C	6.4930517154	-2.6065516181	0.2032142114
H	5.5754923050	-3.1714466754	0.3846718135
H	7.3262149149	-3.1783366247	0.6171347742
H	6.6340968913	-2.5247589093	-0.8755881401
N	-9.0530347912	1.5315963604	2.2949594363
H	-10.0267890071	1.7580932587	2.1902684308
H	-8.4730503363	2.2634156015	2.6625896095
N	-9.9431489206	-1.3153485957	-1.1785979512
H	-10.8650968074	-0.9222831389	-1.1028216207
H	-9.6858954173	-1.6499319938	-2.0891871127
H	10.9620732466	0.1100547365	0.6717152603

DA2 in aqueous phase

C	10.9200447701	1.8463010047	1.3863034300
C	13.1253121113	2.7470499682	1.1457475752
C	12.8954236403	0.5993815335	1.9112961322
N	13.6920392938	1.6150024288	1.5704079987
C	11.5024325500	0.6683737375	1.8370797513
C	11.7424697361	2.9100769721	1.0355368086
H	10.9022969658	-0.1795033992	2.1413084087

H	11.3359598345	3.8386988520	0.6564567409
H	6.9431609233	4.2299239293	1.7302061228
C	7.4233306865	3.2918045103	1.4757475858
C	8.6815969745	0.8725944623	0.8386857626
C	6.6812056247	2.2064517617	1.0350692645
C	8.7998889667	3.1608234368	1.5866013925
C	9.4437861686	1.9616480940	1.2710412321
C	7.3120411249	0.9994479165	0.7193317148
H	9.3858658657	4.0013886916	1.9385430341
H	9.1704702406	-0.0597501759	0.5767571868
C	5.2406526120	2.0525152750	0.7928350149
C	2.6653848333	1.2254619398	0.1059434709
C	4.1785818308	2.9340435540	0.9412195962
C	5.0148713894	0.7580745379	0.3221081696
C	3.7426507047	0.3436768281	-0.0166360307
C	2.9010448831	2.5133246000	0.5970707798
H	4.3357526109	3.9426221131	1.3062226935
H	3.5730984834	-0.6669073661	-0.3730578292
H	2.0725069225	3.2069538559	0.6852349820
C	6.3039363386	-0.0392259918	0.2502007955
C	6.5866516254	-0.5043960654	-1.1830431625
H	7.5458764442	-1.0233056764	-1.2359405308
H	6.6103344201	0.3415958267	-1.8725090096
H	5.8090287827	-1.1960636257	-1.5152406304
C	6.2540067827	-1.2484281078	1.1933338667
H	7.2068657735	-1.7815964270	1.1838838163
H	5.4733141726	-1.9427971549	0.8740374447
H	6.0390256921	-0.9391842359	2.2180493597
H	-0.1898990436	-1.0045438112	-2.7901939040
C	-0.0966359726	-0.3967159450	-1.8972164057
C	0.1654790634	1.1939131288	0.3938912172
C	-1.2158593775	0.0021831329	-1.1841301176
C	1.1536074766	0.0075256204	-1.4571556561
C	1.3054559757	0.8025896835	-0.3164723429
C	-1.0845718780	0.7943272679	-0.0410015872
H	2.0307054073	-0.2812275993	-2.0240714735
H	0.2665849299	1.7984963393	1.2893297429
C	-2.6428987603	-0.2562062356	-1.4136288585
C	-5.4017709715	-0.4149075875	-1.3813173973
C	-3.2899605816	-0.9717861219	-2.4123711952
C	-3.3684245267	0.3782640032	-0.4032911012
C	-4.7502338834	0.3009432572	-0.3817785730
C	-4.6771507703	-1.0457722476	-2.3882485347
H	-2.7293515487	-1.4636051858	-3.1995894617
H	-5.3233851259	0.7907863296	0.3983872610

H	-5.2007030512	-1.5977167124	-3.1604920487
C	-2.4473570933	1.1000991688	0.5645591214
C	-2.5812634061	0.5232592634	1.9785971268
H	-1.8724914459	1.0014309415	2.6575815578
H	-2.3919615978	-0.5520816482	1.9797836403
H	-3.5895472381	0.6943983552	2.3621698437
C	-2.7354276217	2.6058863284	0.5730597970
H	-2.0291890188	3.1282734065	1.2214341106
H	-3.7446272023	2.7956496966	0.9454707839
H	-2.6569345027	3.0230957088	-0.4329565758
N	13.5178659039	-0.5274381288	2.3931324495
H	14.4904006728	-0.6190830613	2.1479078403
H	12.9954840070	-1.3864638191	2.3448282218
N	13.9817196903	3.7792041254	0.8471965631
H	14.9315963222	3.5070566846	0.6524499200
H	13.6247815772	4.5022586616	0.2449657900
H	-6.4838121881	-0.4817536033	-1.3773286925

DA2-CO_2 in gas phase

C	5.8006886793	-0.2649751261	0.0770128927
C	7.7301659460	0.9817421145	-0.5891431148
C	8.0200877574	-0.8447866911	0.7560721829
N	8.5533231260	0.1748427374	0.0818116640
C	6.6489845498	-1.1039639209	0.7847740445
C	6.3456458884	0.8043041299	-0.6191893528
H	6.2607260523	-1.9350815735	1.3592036819
H	5.7205454914	1.4660645849	-1.2049520544
N	8.9028288347	-1.6734949888	1.4011967862
H	9.8281128174	-1.3069771335	1.5422551797
H	8.5415779501	-2.2543232855	2.1349513323
N	8.3179292793	2.0377741173	-1.2417799470
H	9.3034729073	1.9397454173	-1.4167140245
H	7.7907659186	2.4657798611	-1.9809023491
H	2.1539205669	-3.1123977216	-0.2465240953
C	2.5036640452	-2.0945280328	-0.1177138884
C	3.4270743542	0.5272914759	0.1912124743
C	1.6092186512	-1.0467249541	0.0272756148
C	3.8619045226	-1.8234710684	-0.0982807300
C	4.3395603903	-0.5211054362	0.0568511883
C	2.0721356084	0.2617897442	0.1802721638
H	4.5708373310	-2.6327202296	-0.2265061740
H	3.7940960419	1.5389169687	0.3284444908
C	0.1424790354	-1.0299394400	0.0670337770
C	-2.5723619219	-0.4206301012	0.2455256716

C	-0.7940302917	-2.0475334659	-0.0389220341
C	-0.2745025245	0.2877806268	0.2529869466
C	-1.6171488934	0.5935504285	0.3417252228
C	-2.1418127929	-1.7347149473	0.0504087158
H	-0.4874967834	-3.0780510173	-0.1784047322
H	-1.9438844165	1.6205636750	0.4669104761
H	-2.8786894121	-2.5280257925	-0.0047326133
C	0.9105326365	1.2330503385	0.3251566206
C	0.9472066922	1.9631833444	1.6709816402
H	1.8355524339	2.5930176632	1.7476815382
H	0.9578899625	1.2504854499	2.4972304765
H	0.0684702315	2.6022317922	1.7833473250
C	0.8732827903	2.2327889826	-0.8361480914
H	1.7588811864	2.8713356479	-0.8275948056
H	-0.0080647872	2.8738091120	-0.7628706806
H	0.8341016252	1.7101122411	-1.7933036320
C	11.4985388869	0.3170356424	-0.2878498104
O	11.3689053560	0.9635832670	-1.2380151582
O	11.6920744331	-0.3250702142	0.6540195442
H	-6.1112767231	1.8446147519	2.2125617177
C	-5.7944669814	1.1417123725	1.4505763053
C	-4.9557438662	-0.6869155840	-0.4906565941
C	-6.7124123510	0.5582186855	0.5931764288
C	-4.4560475601	0.8075440281	1.3271889975
C	-4.0161952637	-0.0997571694	0.3605529138
C	-6.2917807365	-0.3579762782	-0.3726407753
H	-3.7341480039	1.2411916076	2.0088643763
H	-4.6235497512	-1.3797237589	-1.2571487426
C	-8.1669774706	0.7211306957	0.4804312908
C	-10.8543427354	0.6500322709	-0.1625977109
C	-9.0558683778	1.5084741288	1.1971375018
C	-8.6190654962	-0.0989871251	-0.5544372536
C	-9.9623685684	-0.1382740829	-0.8795440544
C	-10.4033562102	1.4669712050	0.8673096560
H	-8.7108917304	2.1477677282	2.0015192002
H	-10.3237781546	-0.7726482418	-1.6820622971
H	-11.1113858932	2.0759651422	1.4167642176
C	-7.4713486172	-0.8620351649	-1.1931516551
C	-7.6630070325	-2.3752799185	-1.0358079170
H	-6.8061740660	-2.9186039013	-1.4400011376
H	-8.5541209709	-2.7054400167	-1.5748614337
H	-7.7800722664	-2.6479095020	0.0140075290
C	-7.3283257025	-0.4997319780	-2.6760245363
H	-6.4655934817	-1.0032306352	-3.1173040744
H	-7.2025561076	0.5760952518	-2.8055108138

H	-8.2169192475	-0.8079199887	-3.2319497051
H	-11.9096227177	0.6286652331	-0.4082439438

DA2-CO_2 in aqueous phase

C	0.5261852742	2.0854279423	0.5793831890
C	1.2971270388	4.0279103447	-0.6118007545
C	0.2159031107	4.2906431745	1.4877471528
N	0.8280110500	4.8319779384	0.3903012885
C	0.0656626139	2.9149365636	1.5920540852
C	1.1469942591	2.6512615607	-0.5245207888
H	-0.4511300371	2.5226005566	2.4565134376
H	1.5500855217	2.0438203299	-1.3226072673
N	-0.1886970643	5.1193377782	2.4706253844
H	-0.4049040927	6.0731032169	2.2227443451
H	-0.7284760693	4.7072212615	3.2122159295
N	1.8536059432	4.6061297389	-1.6941634030
H	2.2633582991	5.5212535517	-1.5841670404
H	2.2791838473	3.9901731986	-2.3653670976
H	0.3496714447	-1.8981200231	2.9619270747
C	0.2689224253	-1.4083592728	1.9983390498
C	0.0848621824	-0.1272726794	-0.4863738594
C	-0.0046930254	-2.1340497828	0.8483613032
C	0.4394620950	-0.0356484177	1.8989543337
C	0.3493991026	0.6167503648	0.6670136810
C	-0.0934975893	-1.4917803613	-0.3908268924
H	0.6647317293	0.5360845169	2.7910798875
H	-0.0032161340	0.3696817688	-1.4464842371
C	-0.2561334756	-3.5669696097	0.6432978574
C	-0.8607531586	-6.1183211112	-0.3137824182
C	-0.2945654539	-4.6364617799	1.5279510625
C	-0.4995959116	-3.7748307652	-0.7150608743
C	-0.7958771187	-5.0349505578	-1.1935506457
C	-0.5962674361	-5.9015315874	1.0424139553
H	-0.1082068365	-4.4936243490	2.5862330399
H	-0.9733250105	-5.1899543294	-2.2525243852
H	-0.6550420290	-6.7346198754	1.7336296313
C	-0.3968081492	-2.4832363691	-1.5033517210
C	-1.7143073381	-2.1625356533	-2.2182679487
H	-1.6473327003	-1.2015819213	-2.7322230660
H	-2.5454177893	-2.1226417910	-1.5117605020
H	-1.9336883331	-2.9304748708	-2.9635165804
C	0.7488224354	-2.5547810825	-2.5220972170
H	0.8598887775	-1.6004928911	-3.0409786895
H	0.5414200354	-3.3250514099	-3.2684191724
H	1.6944671069	-2.7968209088	-2.0332964660

C	0.9834795922	6.3671344686	0.2755348715
O	2.1196886402	6.7234142808	-0.0125033742
O	-0.0549255752	6.9808255930	0.4899826554
H	-3.3921507275	-8.8712835165	-3.0572763027
C	-2.6198166899	-8.8083598145	-2.2989383031
C	-0.6425797699	-8.6259192471	-0.3229296152
C	-2.0171544064	-9.9508636037	-1.7972271436
C	-2.2266664387	-7.5751037649	-1.8048628071
C	-1.2411149075	-7.4626157775	-0.8185818091
C	-1.0312095617	-9.8593425619	-0.8120200664
H	-2.7098439830	-6.6798348961	-2.1777838484
H	0.1340589668	-8.5552104082	0.4315941563
C	-2.2299452554	-11.3676323745	-2.1175424872
C	-2.2298617900	-14.1234292170	-2.3222026103
C	-3.0948620855	-11.9778414939	-3.0162040901
C	-1.3682738227	-12.1279768803	-1.3245444234
C	-1.3640845472	-13.5086583259	-1.4230302392
C	-3.0877541084	-13.3637383290	-3.1121407333
H	-3.7650454109	-11.3894342523	-3.6330085354
H	-0.6994163788	-14.1093069186	-0.8110203470
H	-3.7560563522	-13.8588699931	-3.8073508756
C	-0.5240226307	-11.2418823746	-0.4250686013
C	-0.7937806790	-11.5482787142	1.0527659080
H	-0.2300509535	-10.8685267535	1.6947740297
H	-0.4894707077	-12.5705467430	1.2882957590
H	-1.8557076858	-11.4449166247	1.2847816867
C	0.9672021657	-11.4068393716	-0.7397305615
H	1.5655817929	-10.7231637269	-0.1343195101
H	1.1676779304	-11.2040616487	-1.7936979559
H	1.2885432831	-12.4273711988	-0.5195244212
H	-2.2373014436	-15.2040232184	-2.4090220669

DA3 in gas phase

H	5.2232018017	-1.8552972137	-0.0942826357
C	5.8778712131	-1.0026168315	-0.0324844361
C	6.3160145833	1.3545665451	-0.0300797422
N	8.1279813314	-0.2050181548	0.1001413325
C	7.6650474436	1.0386602718	0.0378782265
C	7.2459465884	-1.1966004389	0.0748460593
C	5.4039063248	0.3045333606	-0.0758040360
H	6.0088234796	2.3868830102	-0.0375818019
N	7.8443373371	-2.4595772033	0.1503405818
N	8.6874283276	1.9922229162	0.0598229948
H	9.6000634961	1.5792945244	0.1540136127

H	8.8490433549	-2.4128969222	0.1806026538
C	8.6048955513	3.3512181939	-0.0942412421
C	7.2531090497	-3.6895436735	0.2832633866
O	7.5659440377	3.9513917316	-0.2551322929
O	6.0555736835	-3.8675578461	0.2979827925
C	9.9352438329	4.0649348287	-0.0165487277
H	10.7854381955	3.4206896544	-0.2408743405
H	10.0562236070	4.4641092849	0.9921083834
H	9.9179901102	4.9033649001	-0.7093897292
C	8.2307602637	-4.8313624146	0.4460187294
H	7.8042932119	-5.7200758221	-0.0135440779
H	8.3581069123	-5.0303015882	1.5119919721
H	9.2090037235	-4.6259602206	0.0112132346
H	1.7711086706	2.8392922680	-1.4710072189
C	2.1143520828	1.9488625360	-0.9573184458
C	3.0273877385	-0.3526441827	0.3392626004
C	1.2143883823	1.0273043270	-0.4468907596
C	3.4721604630	1.7075703078	-0.8233038930
C	3.9467046295	0.5625561775	-0.1807416973
C	1.6754794297	-0.1225153641	0.1993329937
H	4.1775295343	2.4099587607	-1.2494333950
H	3.3795944006	-1.2399882293	0.8535523148
C	-0.2531010127	0.9857084345	-0.4743771729
C	-2.9637899274	0.3426503276	-0.3180427002
C	-1.1941617847	1.8554526028	-1.0057828590
C	-0.6663199175	-0.1927438086	0.1474169134
C	-2.0054437948	-0.5119257510	0.2301048555
C	-2.5394124336	1.5271400221	-0.9240483708
H	-0.8919274456	2.7714921359	-1.4999779798
H	-2.3257242197	-1.4228275928	0.7249391574
H	-3.2769979433	2.1845272537	-1.3700228776
C	0.5170142032	-1.0037633389	0.6409524297
C	0.5620582154	-2.3735053671	-0.0489627071
H	0.5753644906	-2.2639571546	-1.1344845493
H	-0.3150935485	-2.9659321597	0.2221580075
H	1.4505328669	-2.9327052703	0.2509807115
C	0.4742211233	-1.1786459240	2.1626289465
H	1.3583973963	-1.7133105277	2.5155349155
H	-0.4061472556	-1.7557651794	2.4548952025
H	0.4301775873	-0.2121911365	2.6665375930
H	-6.3534574604	-2.7917401606	-0.7026736817
C	-6.0917915937	-1.7598837419	-0.4982870945
C	-5.3951151997	0.9020839216	0.0021450975
C	-7.0667543483	-0.8211859336	-0.2067800417
C	-4.7674953764	-1.3589443015	-0.5345110722

C	-4.3982457539	-0.0353526853	-0.2814246801
C	-6.7190435393	0.5080697211	0.0385565524
H	-4.0006032665	-2.0819825780	-0.7854383300
H	-5.1181579016	1.9289271758	0.2175135961
C	-8.5229814213	-0.9554261241	-0.0891890500
C	-11.2471397685	-0.6523718717	0.2547219184
C	-9.3502525832	-2.0594900909	-0.2336335568
C	-9.0529658388	0.2958292168	0.2271321878
C	-10.4161132875	0.4524287182	0.3992333536
C	-10.7173935914	-1.8983905251	-0.0590338926
H	-8.9429231973	-3.0341052253	-0.4775716743
H	-10.8403407408	1.4201466925	0.6451617387
H	-11.3786209758	-2.7501487612	-0.1670305710
C	-7.9574549801	1.3424592563	0.3355341461
C	-7.9096000127	1.9391670527	1.7458174138
H	-7.7841488241	1.1547083679	2.4937700791
H	-8.8355178868	2.4751640972	1.9663217401
H	-7.0806408015	2.6430803623	1.8423344053
C	-8.1535754701	2.4432011738	-0.7126041162
H	-9.0817314484	2.9883436496	-0.5266135299
H	-8.2049614473	2.0169113930	-1.7157844069
H	-7.3293080990	3.1586861158	-0.6834875263
H	-12.3170074810	-0.5428424757	0.3880455665

DA3 in aqueous phase

H	-0.1977651599	9.7941304603	-0.1802529126
C	-0.3132459386	10.2813346392	0.7729472053
C	-0.8073086318	10.2648689091	3.1208490060
N	-0.3369510886	12.3285680167	2.0060591282
C	-0.6566898694	11.6453521182	3.1009272305
C	-0.1656516230	11.6581981053	0.8717157499
C	-0.6376213515	9.5734485875	1.9253129511
H	-1.0394814428	9.7595273052	4.0428586249
N	0.1589250736	12.4852693447	-0.2070076853
N	-0.8174418869	12.4663608129	4.2195321370
H	-0.6329168974	13.4390310735	4.0287294319
H	0.1934026433	13.4635058294	0.0350738989
C	-1.2254470942	12.1423701763	5.4802491410
C	0.4563216899	12.1515861787	-1.4967806914
O	-1.5084517579	11.0074231032	5.8271506399
O	0.4580559704	11.0054850288	-1.9149668297
C	-1.2777208056	13.3031263908	6.4384380609
H	-1.3293191834	14.2673774344	5.9354723875
H	-0.3767845207	13.2778993149	7.0550146986
H	-2.1395457011	13.1797396707	7.0917732493

C	0.8214886367	13.3185973434	-2.3762844004
H	0.4456271097	13.1327411362	-3.3806114550
H	1.9107424888	13.3811557331	-2.4257526263
H	0.4350251032	14.2663614274	-2.0049376076
H	-2.6989721155	5.6347326526	3.2723497322
C	-1.9567001152	6.1010548334	2.6346377132
C	-0.0651377725	7.3298171600	0.9748094857
C	-1.2122889750	5.3503903780	1.7374881277
C	-1.7519815531	7.4712666340	2.6923107856
C	-0.8144201027	8.1005857493	1.8692967097
C	-0.2678144553	5.9662103168	0.9109117272
H	-2.3511852511	8.0659535810	3.3711195221
H	0.6747381722	7.8013385027	0.3371072161
C	-1.2332712981	3.9151250855	1.4275631098
C	-0.9016582350	1.3457326956	0.3900104573
C	-1.9953304361	2.8709605082	1.9344378834
C	-0.3024985623	3.6757336418	0.4159324014
C	-0.1300697465	2.4053854608	-0.0954136536
C	-1.8248791625	1.5970933614	1.4101505207
H	-2.7293157407	3.0407022839	2.7141830430
H	0.6048323539	2.2253512581	-0.8726241233
H	-2.4402748856	0.7855584730	1.7816014738
C	0.3990136215	4.9527399659	-0.0062226501
C	0.1114781596	5.2630947684	-1.4812976153
H	-0.9634788989	5.3122398926	-1.6666536028
H	0.5339862268	4.4845516985	-2.1204353808
H	0.5571734646	6.2178496285	-1.7672823337
C	1.9092950349	4.8642648773	0.2344781470
H	2.3932855040	5.8098566153	-0.0174118018
H	2.3448227119	4.0819286275	-0.3911183391
H	2.1250806078	4.6293815848	1.2784849974
H	-0.1710560271	-1.4658669551	-3.2266964200
C	-0.3607618823	-1.3879117646	-2.1620449649
C	-0.8751347648	-1.1643405186	0.5819074254
C	-0.4739881530	-2.5203775585	-1.3717912495
C	-0.5072227958	-0.1438765873	-1.5701924078
C	-0.7576598478	-0.0100119126	-0.2004283359
C	-0.7370305578	-2.4086839734	-0.0046682467
H	-0.4450184475	0.7429651044	-2.1893426147
H	-1.0602892317	-1.0799386523	1.6477273070
C	-0.3742849408	-3.9439215321	-1.7155097062
C	-0.2996592168	-6.7046227038	-1.8095859952
C	-0.1268267218	-4.5716970620	-2.9290292151
C	-0.5830113487	-4.6889643455	-0.5532953117
C	-0.5470757893	-6.0721204285	-0.5950219228

C	-0.0908875377	-5.9599644756	-2.9666804100
H	0.0356204078	-3.9953316490	-3.8330703521
H	-0.7102173203	-6.6609776446	0.3014714174
H	0.1003667086	-6.4686037171	-3.9046951855
C	-0.8393146276	-3.7845128904	0.6398010267
C	0.2258468138	-3.9876167233	1.7225170699
H	1.2275986878	-3.8338194911	1.3163714058
H	0.1694596875	-5.0026496739	2.1220698035
H	0.0735406703	-3.2881078532	2.5468355951
C	-2.2399378546	-4.0274051878	1.2152620716
H	-2.3161342423	-5.0434397187	1.6089709091
H	-3.0039140313	-3.8998950316	0.4455097020
H	-2.4469442317	-3.3292856566	2.0287316328
H	-0.2692817194	-7.7872907720	-1.8562049132

DA3-CO_2 in gas phase

H	5.0124967225	-2.3469711670	0.0246528771
C	5.4268188939	-1.3533069641	0.0671979533
C	5.2239477916	1.0271656233	0.2938087552
C	6.5928096550	1.1027951813	0.0795718903
C	6.7852431765	-1.1610145921	-0.1338998892
C	4.6357164530	-0.2323044545	0.2854602197
H	4.6567095556	1.9239659574	0.4818413230
N	7.6788721365	-2.2062132560	-0.3806830963
N	7.3077272961	2.3024362551	0.0739425067
H	8.2979195107	2.1759170005	-0.0538072422
H	8.6210899678	-1.8980108383	-0.5537509229
C	6.8411303488	3.5869027903	0.1796510134
C	7.4463172555	-3.5580898452	-0.3966286172
O	5.6741091505	3.8766824590	0.3207079931
O	6.3666466332	-4.0656182176	-0.1918770962
C	7.9167493014	4.6444354278	0.0812886631
H	8.9278797630	4.2476384016	0.1686262985
H	7.7452755796	5.3846150627	0.8609000414
H	7.8158459312	5.1467318942	-0.8818823334
C	8.6776698256	-4.3914089062	-0.6710775278
H	8.3947173523	-5.2231712215	-1.3130497247
H	9.0321257758	-4.8047109795	0.2748264603
H	9.4889235676	-3.8286257762	-1.1323997101
H	0.9713344505	-2.4322460593	2.0851733175
C	1.3298868966	-1.6136830042	1.4719896112
C	2.2777853681	0.5015852474	-0.0945186885
C	0.4465257820	-0.7309420521	0.8719134251
C	2.6895449239	-1.4403849564	1.2727877957

C	3.1770356772	-0.3881370591	0.4963615966
C	0.9216717370	0.3210388550	0.0852663871
H	3.3890181539	-2.1254535945	1.7366340127
H	2.6522396644	1.3093638843	-0.7142629202
C	-1.0202829489	-0.6801371937	0.8781873642
C	-3.7284840801	-0.1165891264	0.5349661787
C	-1.9682213681	-1.4922956312	1.4828051304
C	-1.4227028183	0.4027851484	0.0967358146
C	-2.7623533194	0.6866396457	-0.0735652142
C	-3.3129979680	-1.2050348645	1.3050959575
H	-1.6729814228	-2.3390067102	2.0919002768
H	-3.0773977814	1.5162682426	-0.6978913502
H	-4.0603748882	-1.8210736145	1.7920344286
C	-0.2292828896	1.1216115303	-0.5046008579
C	-0.1884427649	2.5907277635	-0.0760232105
H	-0.1894037566	2.6781699993	1.0113535197
H	-1.0592704614	3.1250869591	-0.4626972988
H	0.7067940473	3.0831176350	-0.4605720045
C	-0.2532829909	1.0067630494	-2.0346506468
H	0.6381184151	1.4602870142	-2.4724494257
H	-1.1285651467	1.5171810570	-2.4427907987
H	-0.2949416036	-0.0387930353	-2.3445739129
N	7.3645264128	0.0373845460	-0.1298095036
C	10.4080435089	0.2954047485	-0.5178551089
O	10.3497840564	1.4375444341	-0.3493121405
O	10.5111521894	-0.8429276934	-0.6926781550
H	-7.2766777437	2.8686055842	0.4022073708
C	-6.9542092521	1.8374526672	0.3138188528
C	-6.1004987140	-0.8174051057	0.1145306374
C	-7.8647426189	0.8247433225	0.0614780921
C	-5.6158261922	1.5130786799	0.4640604811
C	-5.1698843276	0.1930786346	0.3685011760
C	-7.4355916269	-0.5001589734	-0.0393997079
H	-4.8994898655	2.2953767610	0.6847642146
H	-5.7616313395	-1.8438902006	0.0173534816
C	-9.3188559721	0.8600600477	-0.1381539230
C	-12.0024457520	0.3566154680	-0.5714803159
C	-10.2171572649	1.9166410991	-0.1239428231
C	-9.7602052665	-0.4442546797	-0.3671114736
C	-11.1011206821	-0.7009990780	-0.5851900651
C	-11.5626079580	1.6547934474	-0.3421466072
H	-9.8812159841	2.9312956170	0.0556769243
H	-11.4537628166	-1.7113811431	-0.7637854468
H	-12.2779188836	2.4686100156	-0.3330123292
C	-8.6048821669	-1.4299932953	-0.3336699815

C	-8.7984417713	-2.4717308411	0.7745038435
H	-9.6816390535	-3.0827364596	0.5736680174
H	-8.9301497632	-1.9924194981	1.7455747490
H	-7.9360597690	-3.1392530847	0.8329138192
C	-8.4419907282	-2.1287467804	-1.6892116865
H	-9.3233367247	-2.7335408949	-1.9155147323
H	-7.5734726247	-2.7907520204	-1.6825508119
H	-8.3139294202	-1.4008758706	-2.4915295131
H	-13.0562545767	0.1681682841	-0.7400159688

DA3-CO_2 in aqueous phase

H	-0.2685461523	-9.4624538962	3.5500889590
C	-0.3797666374	-9.9419803497	2.5921740221
C	-0.4332167726	-9.9060795813	0.2010855826
C	-0.7815437358	-11.2387756687	0.2031966976
C	-0.7094016336	-11.2811980119	2.5592572901
C	-0.2343700044	-9.2371176010	1.4032117829
H	-0.2975741240	-9.4139576039	-0.7468635387
N	-0.8774559346	-12.0410450129	3.6974875512
N	-0.9915038544	-11.9592025994	-0.9553814765
H	-0.8421279298	-12.9580204402	-0.8781817671
H	-1.4870929496	-12.8440008449	3.5960917853
C	-1.4243011968	-11.4644267029	-2.1672970579
C	-0.2613098350	-11.8493048230	4.9161105782
O	-1.6798263220	-10.2928303700	-2.3552207872
O	0.5312993523	-10.9548790716	5.1259716593
C	-1.5953664396	-12.5208377962	-3.2225089819
H	-0.8532751110	-13.3131712017	-3.1304269517
H	-1.5308655043	-12.0574945933	-4.2039455569
H	-2.5870198532	-12.9647846532	-3.1081998305
C	-0.6465181801	-12.8768991108	5.9422760853
H	-0.2505640175	-12.5840635797	6.9106756400
H	-0.2292992026	-13.8447842805	5.6562456341
H	-1.7307785855	-12.9817359562	5.9962192820
H	1.9523844643	-5.5375266079	3.1572975794
C	1.2991027996	-5.9315563903	2.3875192701
C	-0.3678566868	-6.9712930714	0.3902964535
C	0.8052332152	-5.1142878009	1.3802485693
C	0.9489260036	-7.2729045864	2.3925723854
C	0.1201203950	-7.8037073045	1.4009814360
C	-0.0263238909	-5.6365716936	0.3869564775
H	1.3450490953	-7.9232233005	3.1635299180
H	-1.0268066271	-7.3700112061	-0.3735582318
C	0.9890574389	-3.6846851751	1.1148577076
C	0.9775775923	-1.0669314984	0.1772967786

C	1.7166302336	-2.7206814001	1.7948980783
C	0.2665745889	-3.3521278071	-0.0335358664
C	0.2582207863	-2.0534606727	-0.5026341760
C	1.7052274131	-1.4195903016	1.3190683408
H	2.2899800519	-2.9760729076	2.6787527800
H	-0.3207800899	-1.7921685451	-1.3822372829
H	2.2836355088	-0.6620803666	1.8343029213
C	-0.4394400790	-4.5698563718	-0.6097571209
C	0.0750376766	-4.9071959680	-2.0159709867
H	1.1570924354	-5.0517634956	-2.0150503443
H	-0.1671555733	-4.1027100065	-2.7133321328
H	-0.3936016691	-5.8245152044	-2.3797896233
C	-1.9621209107	-4.3940316934	-0.6391669840
H	-2.4398633861	-5.3082227789	-0.9988466720
H	-2.2388848783	-3.5804784509	-1.3126893359
H	-2.3520988801	-4.1703628522	0.3553936151
N	-0.9115082542	-11.9162903548	1.3740073757
C	-1.3014970363	-13.4594132079	1.3535262453
O	-0.5696148099	-14.1117378342	0.6301679295
O	-2.2606195005	-13.7050180940	2.0633530226
H	1.0319598238	2.1708662231	-3.1648653136
C	0.9981844626	1.9576549036	-2.1022925205
C	0.9276502884	1.3847717256	0.6347287075
C	0.9632650428	2.9833275135	-1.1685103170
C	0.9992946764	0.6437595886	-1.6564650017
C	0.9674877217	0.3399463082	-0.2920282172
C	0.9266014954	2.6928022124	0.1952531676
H	1.0456570316	-0.1628566527	-2.3796545863
H	0.8808758077	1.1623380731	1.6953724597
C	0.9556558444	4.4423446873	-1.3288634896
C	0.9240418119	7.1895372212	-1.0703603232
C	0.9839662957	5.2255652815	-2.4734713819
C	0.9116060754	5.0235366563	-0.0581648568
C	0.8957399514	6.3999224318	0.0758151042
C	0.9680134145	6.6073723771	-2.3337181152
H	1.0183801339	4.7707086454	-3.4574966141
H	0.8610346280	6.8624141594	1.0563963979
H	0.9893581437	7.2373227114	-3.2154360515
C	0.8852568411	3.9595775424	1.0272259482
C	2.1140261056	4.0506549422	1.9387938378
H	2.1140181850	4.9922175452	2.4912754297
H	3.0347032956	3.9904099207	1.3547029274
H	2.1108369801	3.2304050253	2.6600209150
C	-0.4047674994	4.0270839754	1.8523608589
H	-0.4598077702	4.9681425975	2.4029611012

H	-0.4364305348	3.2065943408	2.5725825039
H	-1.2820973109	3.9507787382	1.2066085374
H	0.9119042557	8.2693400030	-0.9790988364

C. Trimer-receptors

Trimer in gas phase

H	9.8425643481	-2.6931696876	0.2983714485
C	10.1002963230	-1.6737681941	0.0345388865
C	10.7738915602	0.9591384929	-0.6496051943
C	9.1224760188	-0.6968613024	-0.0682588502
C	11.4212597014	-1.3250309058	-0.2080896169
C	11.7561038534	-0.0196330297	-0.5470200291
C	9.4569547501	0.6163413312	-0.4087607069
H	12.1978927346	-2.0767243350	-0.1326038662
H	11.0449755789	1.9750311240	-0.9161059206
C	7.6678238654	-0.7686787480	0.1255799317
C	4.9259086012	-0.3243786416	0.3762339195
C	6.8312885050	-1.8257123470	0.4524388797
C	7.1352790410	0.5023300850	-0.0876404064
C	5.7799091510	0.7267742430	0.0368859602
C	5.4686441859	-1.5957841704	0.5730904877
H	7.2270943076	-2.8208967453	0.6208519573
H	5.3626373523	1.7112240551	-0.1470834632
H	4.8116806775	-2.4122299120	0.8513773908
C	8.2175652275	1.4950528727	-0.4663074580
C	8.2896958781	2.6430245226	0.5449038536
H	9.1128017636	3.3193769422	0.3062665453
H	8.4405929954	2.2587323138	1.5548853116
H	7.3631640979	3.2216243597	0.5346052571
C	7.9822979871	2.0337421095	-1.8825619418
H	8.7964699663	2.6942169633	-2.1874117719
H	7.0500158578	2.6011771595	-1.9271617059
H	7.9160077593	1.2152168479	-2.6012914088
H	12.7919888956	0.2358381297	-0.7345989083
H	1.3679317291	2.2336638059	1.8901884669
C	1.6836327895	1.3460079268	1.3540978611
C	2.5236813752	-0.9524940946	-0.0008187757
C	0.7558090105	0.4717476107	0.8129902981
C	3.0319333900	1.0649416238	1.2083325031
C	3.4715703147	-0.0745933938	0.5307549519
C	1.1775829838	-0.6772845310	0.1396361895
H	3.7654073173	1.7315305471	1.6457998533

H	2.8540190387	-1.8316766440	-0.5448138471
C	-0.7109860515	0.5071852826	0.8004730476
C	-3.4460174602	0.0577566102	0.4910564364
C	-1.6164604997	1.4183546873	1.3228204653
C	-1.1690112582	-0.6210088391	0.1202837018
C	-2.5211356110	-0.8456507322	-0.0369204536
C	-2.9743604916	1.1863063425	1.1644697570
H	-1.2782501273	2.2962629540	1.8608989086
H	-2.8770727019	-1.7127860974	-0.5836916475
H	-3.6883249757	1.8785302038	1.5957110686
C	-0.0141493637	-1.4776136695	-0.3681850503
H	-7.1152201780	-2.7770911492	0.5477527516
C	-6.7509988166	-1.7666284233	0.4017293851
C	-5.7924289521	0.8361199191	0.0503757892
C	-7.6207863916	-0.7327910249	0.0984149528
C	-5.4000816477	-1.4900736721	0.5266009345
C	-4.9009739104	-0.1970343780	0.3525091907
C	-7.1413242082	0.5664842545	-0.0751928416
H	-4.7162823882	-2.2891832329	0.7874227130
H	-5.4126237203	1.8402799868	-0.1070123396
C	-9.0747552170	-0.7270700023	-0.0989578449
C	-11.7372514015	-0.1591156868	-0.5685572438
C	-10.0069044617	-1.7524271515	-0.0351494928
C	-9.4700040931	0.5777270372	-0.3956896356
C	-10.8015011258	0.8666625758	-0.6317593511
C	-11.3421163875	-1.4583040809	-0.2724009649
H	-9.7050802596	-2.7679542746	0.1949100259
H	-11.1207800166	1.8771155579	-0.8637895111
H	-12.0839341693	-2.2469466899	-0.2264878050
H	-12.7837500444	0.0543063948	-0.7520271868
C	-8.2793727475	1.5205280481	-0.4079938034
C	-0.0678526812	-2.8769596743	0.2568151745
H	0.7983262054	-3.4699236801	-0.0445117095
H	-0.9661176256	-3.4065422170	-0.0695725985
H	-0.0839939208	-2.8193649838	1.3461362520
C	-0.0177556127	-1.5843996746	-1.8978308316
H	0.8469612660	-2.1514075037	-2.2489496414
H	0.0074689963	-0.5964488951	-2.3595862016
H	-0.9184707312	-2.0981510993	-2.2420412282
C	-8.0970305621	2.1507037092	-1.7928839883
H	-7.9981860542	1.3796852082	-2.5586715834
H	-7.2045017217	2.7790043244	-1.8196224706
H	-8.9573965218	2.7741462220	-2.0464073509
C	-8.4345601201	2.6046056850	0.6639569478
H	-7.5502392678	3.2440204845	0.7003206359

H	-8.5774842399	2.1567750825	1.6486870597
H	-9.2997367119	3.2352433516	0.4474622191

Trimer in aqueous phase

H	9.8197363769	-2.7250781468	0.2497481949
C	10.0914934770	-1.7023839326	0.0126861249
C	10.7976741939	0.9442797804	-0.6033156150
C	9.1249247113	-0.7108520679	-0.0748360983
C	11.4190899941	-1.3601027798	-0.2114249688
C	11.7695652006	-0.0484789951	-0.5166846593
C	9.4744796357	0.6079606222	-0.3807563146
H	12.1880303014	-2.1213157596	-0.1481261999
H	11.0790732625	1.9641564532	-0.8429160451
C	7.6671867858	-0.7725872859	0.1043940041
C	4.9263987035	-0.3069432574	0.3360219202
C	6.8180233448	-1.8305730029	0.3994189381
C	7.1495112645	0.5092647504	-0.0846971871
C	5.7941772679	0.7450418932	0.0299110165
C	5.4552851982	-1.5893494195	0.5109742262
H	7.2036544905	-2.8331385847	0.5483403870
H	5.3948703562	1.7404866040	-0.1329197860
H	4.7896549273	-2.4089352409	0.7582668727
C	8.2451136088	1.5012007148	-0.4243217910
C	8.3206471901	2.6185138414	0.6213177119
H	9.1535783188	3.2900947328	0.4047046514
H	8.4591952324	2.2037231354	1.6218114776
H	7.3988636113	3.2045118559	0.6170677589
C	8.0294072787	2.0881873655	-1.8246881051
H	8.8565205866	2.7469063621	-2.0963916608
H	7.1051073839	2.6694552970	-1.8536222774
H	7.9583117094	1.2944654053	-2.5714414724
H	12.8098141562	0.2008597142	-0.6902093558
H	1.3631618275	2.3150492058	1.7416662584
C	1.6806851965	1.4056932434	1.2438756936
C	2.5228325291	-0.9502258723	-0.0171955411
C	0.7539771776	0.5067306431	0.7394423714
C	3.0302287791	1.1192673480	1.1086398823
C	3.4705771798	-0.0488876288	0.4782939795
C	1.1758987464	-0.6697151643	0.1134779925
H	3.7603271348	1.8093485026	1.5145012718
H	2.8479278099	-1.8551736474	-0.5204728808
C	-0.7135008535	0.5385486044	0.7291056260
C	-3.4484832318	0.0695839819	0.4467833775
C	-1.6189469983	1.4707396805	1.2165529963
C	-1.1700495703	-0.6194895786	0.0981349760

C	-2.5228068986	-0.8548385375	-0.0461254785
C	-2.9777942667	1.2284332832	1.0713942363
H	-1.2798028181	2.3719044192	1.7146170901
H	-2.8720607346	-1.7493418074	-0.5513266420
H	-3.6897705919	1.9417496994	1.4707538732
C	-0.0149102137	-1.4943144528	-0.3558346642
H	-7.1061164322	-2.7886758515	0.5062406752
C	-6.7478270352	-1.7743068718	0.3709930251
C	-5.8052912874	0.8420152123	0.0425023108
C	-7.6254549126	-0.7389732023	0.0904106668
C	-5.3957708988	-1.4917717832	0.4840966490
C	-4.9051538217	-0.1922113507	0.3212832274
C	-7.1548519153	0.5658907767	-0.0718334692
H	-4.7073627751	-2.2946715533	0.7203760840
H	-5.4383761976	1.8528416417	-0.1019825889
C	-9.0821713863	-0.7378720728	-0.0923186599
C	-11.7523352050	-0.1765610811	-0.5295849936
C	-10.0079427190	-1.7711372881	-0.0324327215
C	-9.4858237632	0.5699690539	-0.3685009203
C	-10.8219758426	0.8565077675	-0.5885056883
C	-11.3481024021	-1.4794471804	-0.2536871157
H	-9.6971447323	-2.7878019642	0.1816314611
H	-11.1463881532	1.8690326675	-0.8042667911
H	-12.0860357343	-2.2724295287	-0.2112791017
H	-12.8019515011	0.0339938737	-0.7006074751
C	-8.3002563173	1.5189322542	-0.3804795724
C	-0.0629342132	-2.8660968972	0.3291480573
H	0.8052731835	-3.4654780103	0.0473005037
H	-0.9617919638	-3.4080935981	0.0259428545
H	-0.0755452993	-2.7627616091	1.4158760603
C	-0.0222857663	-1.6709210294	-1.8793650428
H	0.8449043184	-2.2509446751	-2.2016679104
H	-0.0026084724	-0.7048606800	-2.3872790183
H	-0.9224629199	-2.2050489402	-2.1923060068
C	-8.1344361646	2.1697277535	-1.7583633133
H	-8.0384833701	1.4104310118	-2.5372601896
H	-7.2451475985	2.8027332791	-1.7792380889
H	-9.0019647800	2.7915512826	-1.9901465677
C	-8.4496222530	2.5908902850	0.7050397381
H	-7.5654275424	3.2305443014	0.7366806059
H	-8.5825123172	2.1326383162	1.6872416131
H	-9.3191596289	3.2186771865	0.4983562604

TA1 in gas phase

C	11.2860702603	-0.4279298476	-0.5012712860
C	11.0889052900	1.5537336591	0.8410336368
N	13.2026363319	0.9951038875	-0.1188143281
C	12.4298736175	1.7841451149	0.6188260897
C	12.6423033881	-0.0770652491	-0.6739075434
C	10.5073691686	0.4174853336	0.2737218686
H	12.9191014307	2.6484304886	1.0581950142
H	10.5025658419	2.2224097822	1.4575117286
C	10.7412232333	-1.6645863205	-1.1786533901
H	10.7090871480	-2.4960760951	-0.4661528662
H	9.7074564182	-1.4927640063	-1.4845776136
C	11.5916111325	-2.0684232684	-2.3780618504
H	11.2729956627	-3.0402739447	-2.7596425398
H	11.4672150924	-1.3406411218	-3.1845795014
C	13.0592657505	-2.1205396318	-1.9846925047
H	13.2123725450	-2.9199251041	-1.2449406752
H	13.6804541488	-2.3565463503	-2.8507627074
N	13.4588044992	-0.8329276387	-1.4702170414
H	14.4332487363	-0.5956155548	-1.4166519277
H	7.0400081065	-2.0870054981	2.0958777192
C	7.3280944465	-1.2305803909	1.4970734866
C	8.0944181514	0.9844961200	-0.0297216724
C	6.3727205941	-0.3851366678	0.9558109691
C	8.6684373847	-0.9649564055	1.2624732320
C	9.0640439930	0.1373327780	0.5059791757
C	6.7570963353	0.7168270941	0.1890122924
H	9.4268249250	-1.6166218007	1.6806696785
H	8.4042329158	1.8376380410	-0.6243706595
C	4.9057381195	-0.4114705635	1.0267975512
C	2.1594937182	0.0439938720	0.8451702146
C	4.0254255246	-1.2871400765	1.6447858547
C	4.4149844429	0.6779082251	0.3071821329
C	3.0578755344	0.9078458272	0.2162089734
C	2.6615964209	-1.0533048726	1.5479053149
H	4.3870793867	-2.1407631652	2.2066950045
H	2.6760066553	1.7452129212	-0.3585331684
H	1.9686638498	-1.7188290824	2.0501776596
C	5.5419210304	1.4744491970	-0.3225497042
C	5.5294154169	2.9301317572	0.1508805396
H	4.6152824251	3.4304622985	-0.1767427079
H	6.3786247541	3.4795269616	-0.2601705394
H	5.5767083421	2.9847455752	1.2394414800
C	5.4526108400	1.4051475690	-1.8529922870
H	4.5355841104	1.8833282211	-2.2046124314

H	5.4463151862	0.3684822290	-2.1939979999
H	6.2999513379	1.9150291051	-2.3157001672
H	-1.4793017461	2.9122202297	1.0371006542
C	-1.1323307678	1.8956419301	0.8915568648
C	-0.2129336711	-0.7229906174	0.5482412406
C	-2.0266820759	0.8625422775	0.6654970373
C	0.2219369454	1.6094166628	0.9449444350
C	0.7012592178	0.3083616961	0.7766925547
C	-1.5641843579	-0.4443816884	0.4928258606
H	0.9267817482	2.4067786147	1.1478277912
H	0.1491058189	-1.7347559619	0.3957428874
C	-3.4912118792	0.8538260206	0.5735259678
C	-6.2051078546	0.2453923624	0.3650817922
C	-4.4296539676	1.8682690416	0.6887626851
C	-3.9060568165	-0.4578874177	0.3433386711
C	-5.2474955843	-0.7626671131	0.2375051334
C	-5.7766919465	1.5561893044	0.5837726368
H	-4.1259044382	2.8917168324	0.8754588445
H	-5.5698334644	-1.7805080421	0.0431828787
H	-6.5175864349	2.3380247374	0.7054370784
C	-2.7215354488	-1.4035538671	0.2498248328
H	-9.8411344615	-2.4294927572	1.4299118289
C	-9.4833858664	-1.5498549769	0.9071727018
C	-8.5410489468	0.7260507440	-0.4158932804
C	-10.3532302647	-0.7394974013	0.1969285165
C	-8.1401440533	-1.2153481850	0.9489499968
C	-7.6502311799	-0.0826748402	0.2946321229
C	-9.8812976495	0.3959493679	-0.4636867772
H	-7.4561398544	-1.8313086202	1.5207671809
H	-8.1667122820	1.5956707067	-0.9461198594
C	-11.7996947467	-0.8449104834	-0.0285896339
C	-14.4487874995	-0.5691298264	-0.7632430686
C	-12.7233798860	-1.7849612697	0.4040815111
C	-12.1966429991	0.2283262184	-0.8273949428
C	-13.5214305489	0.3707066014	-1.1971707541
C	-14.0518232103	-1.6390205967	0.0300599188
H	-12.4197956905	-2.6226742416	1.0214746321
H	-13.8413742057	1.2006136145	-1.8182928112
H	-14.7868261406	-2.3644702154	0.3583193739
H	-15.4898902845	-0.4693261558	-1.0470793072
C	-11.0141443482	1.1111926796	-1.1861646309
C	-2.8017026160	-2.4922461799	1.3262900501
H	-3.6768093930	-3.1257204486	1.1626473581
H	-2.8805167083	-2.0543773145	2.3223694916
H	-1.9169462930	-3.1319550055	1.2993280106

C	-2.6407584260	-2.0445323380	-1.1413340602
H	-3.5194064189	-2.6670131675	-1.3263547448
H	-1.7556671897	-2.6787004231	-1.2249860310
H	-2.5937591725	-1.2830553560	-1.9209766892
C	-11.2106996353	2.5354137452	-0.6568456872
H	-12.0708655041	3.0072949126	-1.1372794755
H	-10.3316487422	3.1499164626	-0.8618402577
H	-11.3838593291	2.5284939348	0.4203142938
C	-10.7901338582	1.1272056837	-2.7029003025
H	-11.6440600227	1.5811305303	-3.2110062772
H	-10.6652748002	0.1138914854	-3.0879343447
H	-9.8994663221	1.7046585881	-2.9587690555

TA1 in aqueous phase

C	-9.7824229888	-5.1350444202	2.8363882501
C	-9.6422084508	-5.7074308707	0.5039240481
N	-11.6725924818	-6.1264657418	1.6883604690
C	-10.9379927449	-6.1616213695	0.5768377179
C	-11.1143147843	-5.6165831774	2.7898148288
C	-9.0469070756	-5.1895282451	1.6628540169
H	-11.4224867977	-6.5814691949	-0.3003395968
H	-9.0876193811	-5.7668623123	-0.4236790415
C	-9.2543382551	-4.5617438527	4.1302870846
H	-8.6858993944	-5.3268822280	4.6687294129
H	-8.5538469916	-3.7528611265	3.9153692349
C	-10.3853342151	-4.0645342735	5.0236276568
H	-9.9955260074	-3.7725255280	5.9996446162
H	-10.8543114494	-3.1830413140	4.5765795970
C	-11.4316101063	-5.1521557902	5.1914650235
H	-10.9971904685	-6.0034468672	5.7316443736
H	-12.2793492666	-4.7906377043	5.7746519206
N	-11.9164851391	-5.5512648800	3.8878814196
H	-12.7957580846	-6.0342210320	3.8189200150
H	-4.5669870031	-5.3341017990	2.9129351418
C	-5.3255938780	-4.8783921534	2.2866641555
C	-7.2937885506	-3.7328723806	0.6565466960
C	-4.9959671273	-3.8949737378	1.3652975208
C	-6.6495169165	-5.2793813220	2.3909981696
C	-7.6393644194	-4.7164894541	1.5841293784
C	-5.9785387861	-3.3233572241	0.5558465983
H	-6.9205929847	-6.0559427531	3.0968346306
H	-8.0616338629	-3.2980553890	0.0244793044
C	-3.7084174762	-3.2822845428	1.0245845155
C	-1.5736573776	-1.8100065059	0.0137595704
C	-2.4342438449	-3.5129882615	1.5175352111

C	-3.9205435064	-2.3346639769	0.0204645810
C	-2.8654876425	-1.5970886350	-0.4788144634
C	-1.3775103986	-2.7784891155	1.0037859097
H	-2.2601540430	-4.2609270836	2.2828338094
H	-3.0382546724	-0.8439394513	-1.2402373882
H	-0.3756532006	-2.9713829801	1.3680404448
C	-5.3868447124	-2.2892001942	-0.3851854257
C	-5.5725531005	-2.7174999434	-1.8478420628
H	-5.0880519572	-2.0057232616	-2.5194645673
H	-6.6350853307	-2.7526973898	-2.0993751792
H	-5.1456073439	-3.7067308987	-2.0244698212
C	-6.0097174010	-0.9071631088	-0.1622866767
H	-5.5322938885	-0.1643346867	-0.8046328254
H	-5.9014442773	-0.5900213159	0.8765023367
H	-7.0744060348	-0.9303077000	-0.4058090662
H	0.7227354079	0.4110484233	-3.3696191058
C	0.7016506759	0.1109723076	-2.3278745652
C	0.6316613081	-0.6840301516	0.3522345530
C	1.7414617284	0.4375599364	-1.4692142541
C	-0.3695833928	-0.6208234434	-1.8370069243
C	-0.4233651759	-1.0255103559	-0.4992773316
C	1.7046796316	0.0341687275	-0.1342157023
H	-1.1726463440	-0.8984259691	-2.5102213182
H	0.5972128075	-0.9732586085	1.3969415497
C	2.9837553113	1.1843851972	-1.6896285132
C	5.4311816177	2.4999791746	-1.5517884794
C	3.4870699161	1.7975066039	-2.8266417761
C	3.6952076558	1.2225131552	-0.4880181577
C	4.9107420158	1.8731428797	-0.4153691669
C	4.7071879992	2.4510279369	-2.7472432578
H	2.9438323024	1.7655964615	-3.7647536773
H	5.4549030833	1.9168229020	0.5221488885
H	5.1162775859	2.9189014329	-3.6353055057
C	2.9472104788	0.4844570302	0.6105295486
H	9.8391127809	2.9129054778	-0.1277497344
C	9.0219141448	3.3422287188	-0.6966298675
C	6.9055528052	4.4182393532	-2.1771944786
C	9.1789535254	4.5380203555	-1.3826528513
C	7.7990453913	2.6897687777	-0.7579203987
C	6.7309345351	3.2126343252	-1.4931336863
C	8.1207543742	5.0702193664	-2.1200090162
H	7.6740677498	1.7442683778	-0.2424169483
H	6.0800969163	4.8430204731	-2.7389453927
C	10.3305370163	5.4386579921	-1.5149353899
C	12.1506314776	7.4320953868	-2.0912849357

C	11.6108486444	5.3524454662	-0.9887881182
C	9.9569665118	6.5124444103	-2.3287708034
C	10.8652088413	7.5141245549	-2.6191192047
C	12.5201976792	6.3598478719	-1.2847363968
H	11.8981724533	4.5155514984	-0.3618627867
H	10.5857625978	8.3516530144	-3.2495020266
H	13.5262638417	6.3105883015	-0.8849279114
H	12.8721773796	8.2100749329	-2.3116798341
C	8.5155065148	6.3711814315	-2.7930352080
C	3.7468250234	-0.7270075282	1.1052791024
H	4.6770988268	-0.4053252280	1.5775010861
H	3.9918454580	-1.3933853259	0.2754992690
H	3.1663348122	-1.2908822228	1.8387180345
C	2.5904036194	1.4100409128	1.7773250888
H	3.4951570342	1.7772712114	2.2656069282
H	1.9960261161	0.8723734462	2.5191744460
H	2.0113645127	2.2676892082	1.4288009223
C	8.4250308385	6.2440438082	-4.3192320045
H	8.7735452861	7.1596261017	-4.8013937879
H	7.3899124063	6.0719645978	-4.6230872336
H	9.0307738361	5.4098783050	-4.6789456081
C	7.6413654533	7.5334370562	-2.3085588899
H	7.9746826613	8.4741084975	-2.7515091762
H	7.6825904325	7.6271908812	-1.2216679263
H	6.6012677056	7.3703077439	-2.5999736149

TA1-CO_2 in gas phase

C	10.2817146579	-0.5356558712	-0.2940023926
C	10.4211592897	1.5263174740	0.9327227400
N	12.3857153862	0.2071575292	0.6378449896
C	11.7628870087	1.2801210002	1.1151364429
C	11.6680750738	-0.6748665084	-0.0576204335
C	9.6603275082	0.5943154799	0.2187760583
H	12.3825450067	1.9709975678	1.6786140419
H	9.9570122762	2.4075314276	1.3551242151
C	9.5672151050	-1.5887483535	-1.1114484412
H	9.0748537180	-2.3079832851	-0.4476374546
H	8.7710388639	-1.1261598867	-1.6973381004
C	10.5287688531	-2.3447300220	-2.0213253006
H	10.0179906842	-3.1823292150	-2.4999231374
H	10.8916718023	-1.6835964333	-2.8128935064
C	11.7145317468	-2.8502385296	-1.2170033107
H	11.3722545021	-3.6006888568	-0.4897365549
H	12.4420540685	-3.3388969560	-1.8676087632

N	12.3590019689	-1.7359023036	-0.5662506157
H	13.3092653337	-1.8221922614	-0.2504607618
H	6.1145203335	3.2109399711	-1.2372185629
C	6.4269699450	2.2846785907	-0.7689434581
C	7.2597097079	-0.1025628219	0.4236669065
C	5.4980878573	1.3333186599	-0.3802410379
C	7.7749983693	2.0301146493	-0.5633764656
C	8.2068474201	0.8405702615	0.0229836401
C	5.9181162400	0.1421489685	0.2172666891
H	8.5135479852	2.7572297761	-0.8797610624
H	7.5865375217	-1.0217621328	0.8977408985
C	4.0337468721	1.3014186676	-0.4940922825
C	1.3140118262	0.6757500911	-0.5109362282
C	3.1257843238	2.2109979947	-1.0157686449
C	3.5823596325	0.0889636028	0.0277135566
C	2.2389433413	-0.2231980472	0.0232440793
C	1.7758884075	1.8914277804	-1.0196223342
H	3.4577712367	3.1546054544	-1.4329496494
H	1.8878066777	-1.1603611495	0.4425000095
H	1.0645676679	2.5839605143	-1.4549317289
C	4.7342440038	-0.7581206267	0.5357621903
C	4.8153536992	-2.0832085104	-0.2331092605
H	3.9242054614	-2.6874607989	-0.0475247790
H	5.6851697091	-2.6636295508	0.0823165246
H	4.8894806306	-1.9081995541	-1.3075672022
C	4.6049838412	-1.0262989626	2.0389685374
H	3.7091558053	-1.6164045104	2.2457985546
H	4.5337100396	-0.0924800193	2.5980437542
H	5.4675885424	-1.5847613017	2.4084611219
C	15.0596110458	-0.1046539087	1.4226120834
O	15.0343914347	0.9181381699	1.9578485426
O	15.1641576387	-1.1399413045	0.9112171367
H	-2.1165029580	-2.3535179079	-1.2514359239
C	-1.8428658119	-1.3462937597	-0.9587923965
C	-1.1144324580	1.2535329530	-0.2301513550
C	-2.8105733527	-0.4116650582	-0.6305530367
C	-0.5103083746	-0.9725432076	-0.9175911722
C	-0.1258752991	0.3201120931	-0.5528095670
C	-2.4454739195	0.8865562239	-0.2682400563
H	0.2516791474	-1.6909455978	-1.1958997045
H	-0.8256542576	2.2546611178	0.0726883483
C	-4.2725680577	-0.5170274556	-0.5823462161
C	-7.0259308456	-0.1480531838	-0.3437315663
C	-5.1286226251	-1.5744226857	-0.8511040269
C	-4.7872867849	0.7177238572	-0.1891630626

C	-6.1492421400	0.9033806472	-0.0665872077
C	-6.4960158913	-1.3808616317	-0.7313569655
H	-4.7457119710	-2.5390625224	-1.1644252012
H	-6.5494647965	1.8573521565	0.2602655071
H	-7.1721269597	-2.1938755128	-0.9701519393
C	-3.6760590169	1.7232074857	0.0525187898
H	-10.8494341809	2.3940238657	-1.0027285020
C	-10.4304035049	1.4636650901	-0.6367962231
C	-9.3274744737	-0.9380744685	0.2733535638
C	-11.2438135859	0.4711652624	-0.1159704753
C	-9.0643995957	1.2447224267	-0.7023211440
C	-8.4929307265	0.0529103220	-0.2502417672
C	-10.6909925296	-0.7288595925	0.3349662450
H	-8.4255651153	2.0027142800	-1.1392565463
H	-8.8950851273	-1.8618673004	0.6439228230
C	-12.6995438616	0.4104271625	0.0627777909
C	-15.3341160362	-0.2316020424	0.5993943096
C	-13.6946587483	1.3303309339	-0.2326867945
C	-13.0196724423	-0.8275284578	0.6224150929
C	-14.3359508597	-1.1528380087	0.8931437103
C	-15.0147664095	0.9996678907	0.0396053478
H	-13.4529706906	2.2914449112	-0.6716257289
H	-14.5952991782	-2.1128030076	1.3271326398
H	-15.8047402016	1.7060628591	-0.1863355879
H	-16.3696564289	-0.4752870811	0.8059893148
C	-11.7750425276	-1.6700996149	0.8420545628
C	-3.6746495996	2.1929663456	1.5108670757
H	-4.5982190282	2.7288524304	1.7410860084
H	-2.8364745145	2.8658332772	1.7023215029
H	-3.5966566982	1.3430940013	2.1907435207
C	-3.8081614752	2.9145158251	-0.9021222310
H	-4.7334799894	3.4610207283	-0.7060595984
H	-3.8254783234	2.5778552470	-1.9399964234
H	-2.9737435741	3.6076033267	-0.7779873521
C	-11.5904662800	-2.0104656579	2.3244860778
H	-12.4160310781	-2.6321833558	2.6786969993
H	-11.5609106524	-1.1052730598	2.9323964642
H	-10.6621500144	-2.5632892159	2.4827846404
C	-11.8333552668	-2.9554409218	0.0063714018
H	-11.9773087023	-2.7279956721	-1.0509794712
H	-12.6622416091	-3.5875987716	0.3335390276
H	-10.9105351629	-3.5295937589	0.1129713116

TA1-CO_2 in aqueous phase

C	-9.2004370607	-5.5398418291	1.3292924847
C	-9.3356518032	-4.4838527032	3.4874061455
N	-11.2673898380	-5.5633955949	2.5942913608
C	-10.6531829595	-4.8707183204	3.5531779104
C	-10.5576018159	-5.9005822766	1.5146555086
C	-8.5922746407	-4.8160263463	2.3456045923
H	-11.2622343154	-4.6100323597	4.4138046468
H	-8.8894690972	-3.9104255065	4.2892978573
C	-8.4919266307	-5.9741507753	0.0650490545
H	-8.4875756123	-5.1503709073	-0.6556959498
H	-7.4454283257	-6.1934172039	0.2842258788
C	-9.1645389413	-7.1799109790	-0.5810925260
H	-8.7260109109	-7.3724649656	-1.5613534505
H	-9.0105477424	-8.0724520770	0.0319303239
C	-10.6542220264	-6.9268263823	-0.7229430753
H	-10.8244831196	-6.0890959440	-1.4123756142
H	-11.1610255949	-7.7998536770	-1.1360659333
N	-11.2125977324	-6.6556611324	0.5850455229
H	-12.2115203063	-6.6991719753	0.6962114298
H	-4.3066531344	-4.4315104479	4.0926351521
C	-4.9782769325	-4.2046333600	3.2723796364
C	-6.7278026764	-3.6349809013	1.1607835561
C	-4.5442990653	-3.4812688886	2.1713236009
C	-6.2955057633	-4.6401687518	3.3080036760
C	-7.1780703825	-4.3650402401	2.2613490299
C	-5.4179515935	-3.2027588562	1.1189665320
H	-6.6483569517	-5.2125232688	4.1583967367
H	-7.4099447088	-3.4017446280	0.3506933743
C	-3.2401765480	-2.8910305975	1.8511843493
C	-1.0361870328	-1.5816015617	0.7767265243
C	-2.0542869399	-2.8654797247	2.5677932412
C	-3.3300916262	-2.2728443596	0.6013247701
C	-2.2363511714	-1.6252533923	0.0615368538
C	-0.9618822842	-2.2072745619	2.0245966286
H	-1.9764487291	-3.3514806664	3.5336786629
H	-2.3097272316	-1.1313669928	-0.9020133432
H	-0.0258025198	-2.1892154286	2.5703939502
C	-4.7252351676	-2.4260768239	0.0137056687
C	-4.7044166996	-3.2381817204	-1.2888070510
H	-4.1470736115	-2.7060072895	-2.0626284104
H	-5.7228706057	-3.3952745919	-1.6519736206
H	-4.2407150518	-4.2147107955	-1.1366358951
C	-5.3983420747	-1.0703408642	-0.2286916257
H	-4.8547319599	-0.5045443140	-0.9882157222

H	-5.4331014561	-0.4777625993	0.6872872536
H	-6.4212650292	-1.2150679565	-0.5839323762
C	-14.1971525520	-5.0990190605	2.4903992894
O	-14.1607773866	-4.6397017262	3.5501720503
O	-14.2789771529	-5.5493620703	1.4275614723
H	1.8730765923	-0.4780037109	-2.6806110992
C	1.6122684376	-0.3584511185	-1.6349835649
C	0.9314942613	-0.0737859064	1.0644632477
C	2.3837421161	0.4285310695	-0.7918738911
C	0.4968848155	-1.0009258720	-1.1174701125
C	0.1475067365	-0.8749877007	0.2300227679
C	2.0371376911	0.5741421273	0.5518898620
H	-0.1049157751	-1.6291846904	-1.7649072391
H	0.6539392164	0.0493324244	2.1060443131
C	3.5920212648	1.2200487069	-1.0431774005
C	5.8314547937	2.8699473214	-0.9709353863
C	4.3321652084	1.4070030089	-2.2002738125
C	3.9647976486	1.8480649536	0.1474970307
C	5.0752646469	2.6678348158	0.1876644309
C	5.4467925479	2.2299376001	-2.1536040075
H	4.0528403066	0.9171793817	-3.1266784134
H	5.3508423203	3.1730075470	1.1073521131
H	6.0407106546	2.3677327519	-3.0496984285
C	2.9974256988	1.5044952706	1.2690097291
H	9.6711671208	4.5753100579	1.0270706553
C	9.0097495438	4.5865759930	0.1678752085
C	7.2980077687	4.5832776757	-2.0450282716
C	9.2718421332	5.3997807525	-0.9254080474
C	7.8874438732	3.7707116666	0.1437044025
C	7.0224038850	3.7544484626	-0.9545970203
C	8.4137891677	5.3951365920	-2.0262419176
H	7.6876100143	3.1167342445	0.9847809812
H	6.6259771641	4.5951412965	-2.8968989242
C	10.3630927870	6.3439689605	-1.1984552204
C	12.1509799322	8.1918318193	-2.2081863870
C	11.4654878501	6.7006699580	-0.4359418336
C	10.1521086720	6.9053886465	-2.4616163734
C	11.0438951745	7.8316377544	-2.9709284546
C	12.3595668561	7.6303561642	-0.9521033752
H	11.6289689015	6.2623133222	0.5422246698
H	10.8885840627	8.2721622040	-3.9502076793
H	13.2278733865	7.9206285604	-0.3722263575
H	12.8582843407	8.9153157567	-2.5966687531
C	8.8888571087	6.3534507488	-3.1030284081
C	2.2645364415	2.7530535561	1.7740467460

H	2.9683645074	3.4540388004	2.2269904040
H	1.5220701956	2.4781329222	2.5263400532
H	1.7511623970	3.2590833563	0.9536494055
C	3.7038005095	0.7878221198	2.4239249207
H	4.4376948679	1.4470995928	2.8914495831
H	4.2179799335	-0.1070585022	2.0674903855
H	2.9788900683	0.4884246947	3.1839177333
C	7.8542449444	7.4558055627	-3.3605488101
H	8.2349533540	8.1735746808	-4.0902737737
H	7.6135812997	7.9914648773	-2.4403623308
H	6.9329419526	7.0244090800	-3.7585523396
C	9.1954732507	5.6089416458	-4.4089585893
H	9.9235976311	4.8119728256	-4.2459814517
H	9.5965685714	6.2972390097	-5.1558997402
H	8.2835936650	5.1637145525	-4.8135413589

TA2 in gas phase

C	-10.7860115783	0.1113119374	0.5720218450
C	-13.1291521264	-0.2696827139	0.2888807180
C	-12.4587304242	1.5371325609	1.5125544103
N	-13.4470568500	0.8098406614	0.9984671341
C	-11.1092733087	1.2322682869	1.3249277353
C	-11.8116736906	-0.6596220537	0.0428037177
H	-10.3396093039	1.8313274054	1.7941095848
H	-11.6000540097	-1.5299102005	-0.5649920843
H	-7.3494743374	-2.9976917264	0.3024738332
C	-7.6442786483	-1.9576463590	0.2223792914
C	-8.4217536820	0.7212112842	0.0464598180
C	-6.7134714294	-0.9726122411	-0.0678509636
C	-8.9660338775	-1.5935259484	0.4224455840
C	-9.3691552257	-0.2596992238	0.3417062322
C	-7.1052766523	0.3626341567	-0.1582772928
H	-9.7000379856	-2.3510540680	0.6713354137
H	-8.7379089177	1.7554591750	-0.0387575622
C	-5.2710195771	-1.0475985046	-0.3122351973
C	-2.5612658853	-0.6208236226	-0.7694180899
C	-4.4087594393	-2.1309550751	-0.3305108105
C	-4.7929964088	0.2428486616	-0.5449776051
C	-3.4485596779	0.4586820362	-0.7675758478
C	-3.0620513469	-1.9085100256	-0.5626507087
H	-4.7762001965	-3.1383698200	-0.1702376817
H	-3.0676379659	1.4641811706	-0.9110720871
H	-2.3828693213	-2.7520469826	-0.5986450350
C	-5.9278750164	1.2549367746	-0.5047154826

C	-6.1340345498	1.8990889064	-1.8816739083
H	-7.0019699014	2.5621890357	-1.8689089943
H	-6.3015840471	1.1354841355	-2.6432137111
H	-5.2602493569	2.4868839640	-2.1700477696
C	-5.7092509532	2.3242388975	0.5677903490
H	-6.5697241997	2.9952138312	0.6180740306
H	-4.8258397794	2.9252882369	0.3437320219
H	-5.5755948597	1.8662835785	1.5490132177
H	1.0666679366	1.5297314836	-2.7279133612
C	0.7233598168	0.7825914162	-2.0214838532
C	-0.1863876161	-1.1487082616	-0.2214284978
C	1.6245947008	0.0415365441	-1.2729131694
C	-0.6338063625	0.5508052035	-1.8620489165
C	-1.1080591166	-0.4043204898	-0.9602435425
C	1.1650793129	-0.9288186353	-0.3832705525
H	-1.3443586855	1.1084623548	-2.4612758886
H	-0.5446843106	-1.8788479492	0.4964962762
C	3.0880141817	0.0702064963	-1.2055061914
C	5.7936267365	-0.2462950273	-0.6485789944
C	4.0125802962	0.8601123740	-1.8676675135
C	3.5081103829	-0.8876074403	-0.2802312240
C	4.8500829813	-1.0487457148	-0.0030121061
C	5.3578172680	0.6955687996	-1.5829403138
H	3.6944368422	1.5947975606	-2.5985681035
H	5.1800786436	-1.7713513278	0.7361708387
H	6.0921722385	1.2971685905	-2.1055877035
C	2.3184370171	-1.6321455000	0.3084247383
H	9.6396845000	-2.7183110427	0.1997235459
C	9.1883514453	-1.7369571832	0.1081817063
C	8.0071195449	0.7805146591	-0.1503220899
C	9.9412009807	-0.5865266786	0.2862595390
C	7.8412557687	-1.6189721819	-0.1974463623
C	7.2355017931	-0.3682858737	-0.3313118066
C	9.3466164054	0.6678541258	0.1573555003
H	7.2475776866	-2.5119338577	-0.3580411881
H	7.5352223214	1.7543779757	-0.2285314797
C	11.3571314901	-0.3934433909	0.6186754616
C	13.8900748890	0.5136972225	1.2285366642
C	12.3655402760	-1.3155543911	0.8483166307
C	11.6087777512	0.9787568964	0.6927673507
C	12.8760238708	1.4368121143	0.9982007544
C	13.6364017312	-0.8506958352	1.1544333679
H	12.1680878829	-2.3801810653	0.7921270056
H	13.0840931550	2.4995587058	1.0600179669
H	14.4375375567	-1.5566752575	1.3376457719

H	14.8877525240	0.8602921711	1.4694702579
C	10.3469893057	1.7789224088	0.4104774286
C	2.2354588495	-1.4783718343	1.8294723732
H	1.3356218586	-1.9640614095	2.2139764514
H	2.2018097856	-0.4257600971	2.1136479154
H	3.0981247270	-1.9397053345	2.3143698124
C	2.3458763581	-3.1174074336	-0.0772979859
H	1.4469262629	-3.6224396681	0.2840526582
H	3.2128165595	-3.6164444600	0.3606925759
H	2.3903573101	-3.2375940110	-1.1609420245
C	9.9315762123	2.6158873797	1.6257254694
H	8.9821561143	3.1217768646	1.4362654193
H	10.6822335421	3.3769024817	1.8479778108
H	9.8097147806	1.9841728123	2.5070896927
C	10.5005732698	2.6652532667	-0.8295812850
H	9.5599606713	3.1734619498	-1.0542563202
H	10.7812198526	2.0687929323	-1.6991270310
H	11.2665365688	3.4271803400	-0.6719850015
N	-12.8456422697	2.6039424442	2.2891287096
H	-13.8084344830	2.8727341683	2.1838216695
H	-12.1921711253	3.3566638545	2.4042615122
N	-14.1888203138	-1.0129980184	-0.1762599683
H	-15.0746184175	-0.5381606520	-0.1631536383
H	-14.0258821500	-1.6085721669	-0.9675001522

TA2 in aqueous phase

C	-10.8433266010	0.1552143872	0.5013712111
C	-13.1655824557	-0.3767560673	0.2589911034
C	-12.5912813620	1.7073643968	1.0200815309
N	-13.5415625855	0.8333764252	0.6792499865
C	-11.2272686099	1.4141040357	0.9476662319
C	-11.8271113128	-0.7610371748	0.1506729283
H	-10.4984409412	2.1524278470	1.2557616547
H	-11.5768083673	-1.7455278758	-0.2228539542
H	-7.3229230160	-2.8561593194	0.8740725560
C	-7.6392991709	-1.8518380582	0.6158518062
C	-8.4726593304	0.7425335217	-0.0282233306
C	-6.7233355142	-0.9009813658	0.1898301341
C	-8.9760484224	-1.4959485546	0.7128173286
C	-9.4072666726	-0.2050635688	0.3953173671
C	-7.1414251513	0.3914716889	-0.1294175995
H	-9.6981051013	-2.2275433495	1.0567712614
H	-8.8014652721	1.7415066438	-0.2938231710
C	-5.2738072918	-0.9778808774	-0.0115528286
C	-2.5650003078	-0.5647428831	-0.5036045795

C	-4.3890167387	-2.0327749485	0.1468855670
C	-4.8193872946	0.2719041143	-0.4376574473
C	-3.4757715861	0.4835321769	-0.6739510205
C	-3.0437981514	-1.8181842089	-0.1066895756
H	-4.7376441720	-3.0117247348	0.4570301933
H	-3.1243495258	1.4650279517	-0.9727169324
H	-2.3521238792	-2.6456925342	-0.0041922235
C	-5.9751967976	1.2497640912	-0.5820449337
C	-6.1571574977	1.6729609593	-2.0458453287
H	-7.0386140681	2.3096675259	-2.1487843794
H	-6.2883518180	0.7997701242	-2.6885381806
H	-5.2868712647	2.2323861381	-2.3944057174
C	-5.8104319348	2.4779433660	0.3168330375
H	-6.6876043976	3.1239643263	0.2382477513
H	-4.9334907026	3.0565493411	0.0202371117
H	-5.6949578615	2.1815340135	1.3612397530
H	1.0362178850	1.5112721298	-2.6008426307
C	0.7040947508	0.7923860409	-1.8601832878
C	-0.1766389837	-1.0651974374	0.0349189146
C	1.6174822956	0.0804477337	-1.0960643031
C	-0.6511847854	0.5652983365	-1.6705700641
C	-1.1121927679	-0.3523448072	-0.7208499484
C	1.1725664571	-0.8545775718	-0.1612952555
H	-1.3664801756	1.1030742016	-2.2820100874
H	-0.5132136923	-1.7708651005	0.7865003279
C	3.0825598927	0.1056200034	-1.0581112310
C	5.7980994069	-0.2153983700	-0.5536022236
C	3.9964627435	0.8695064331	-1.7666640740
C	3.5163538214	-0.8245451393	-0.1099178192
C	4.8639304071	-0.9898718478	0.1409136166
C	5.3478334867	0.7035504754	-1.5062511372
H	3.6654808066	1.5838080177	-2.5123251683
H	5.2007808168	-1.6981077398	0.8908259870
H	6.0714419010	1.2891476005	-2.0613986361
C	2.3361974163	-1.5408966234	0.5299206338
H	9.6200211876	-2.7144256607	0.3411042579
C	9.1858576678	-1.7313247918	0.1970157721
C	8.0493947068	0.7951821215	-0.1943107209
C	9.9673504373	-0.5873019563	0.2734819677
C	7.8310148961	-1.6014635247	-0.0728984226
C	7.2482204916	-0.3466905071	-0.2723390471
C	9.3962781630	0.6706533538	0.0799505843
H	7.2142714425	-2.4904026813	-0.1461209005
H	7.6022242390	1.7747804270	-0.3272895680
C	11.3974953261	-0.4061645141	0.5498217698

C	13.9682802676	0.4791972663	1.0196823311
C	12.3926666159	-1.3378535035	0.8055651009
C	11.6793317720	0.9629365457	0.5279232487
C	12.9663525345	1.4111144855	0.7633168059
C	13.6838005614	-0.8829373925	1.0406816626
H	12.1692009885	-2.3990377838	0.8223306227
H	13.1970486863	2.4710051088	0.7500214717
H	14.4762116459	-1.5943480788	1.2421737589
H	14.9809633948	0.8172357453	1.2057391243
C	10.4268927479	1.7725522669	0.2318027471
C	2.2883740011	-1.3373434368	2.0469174575
H	1.3937855104	-1.8067379901	2.4624365127
H	2.2672144748	-0.2753297634	2.2985411482
H	3.1604546477	-1.7905373825	2.5223722584
C	2.3467215571	-3.0392944267	0.1957165548
H	1.4524603580	-3.5216867741	0.5970017695
H	3.2218902556	-3.5238936651	0.6332284100
H	2.3657229393	-3.1984780028	-0.8844159818
C	10.0644002582	2.6946132936	1.4020859876
H	9.1227403703	3.2099253551	1.1999926633
H	10.8403408462	3.4476626754	1.5529117216
H	9.9508562230	2.1230593257	2.3255961831
C	10.5619952772	2.5778263313	-1.0648929242
H	9.6237961892	3.0896727703	-1.2906458330
H	10.8064127489	1.9239524674	-1.9045293380
H	11.3472414270	3.3303522803	-0.9701812776
N	-13.0280546893	2.9176001726	1.5019133827
H	-13.9764004032	3.1582700725	1.2632440409
H	-12.3789472348	3.6852307994	1.4568108055
N	-14.1772332779	-1.2595404997	-0.0332102025
H	-15.0738322248	-0.8424203184	-0.2236499369
H	-13.9439990317	-2.0363770194	-0.6289772795

TA2-CO_2 in gas phase

C	9.9722606730	-0.1226576148	-0.0628720426
C	11.7814700820	1.1679614917	-0.9471565131
C	12.2604084551	-0.5392025959	0.4970502083
N	12.6906488608	0.4539106213	-0.2824275747
C	10.9104241049	-0.8641680564	0.6402583231
C	10.4101502843	0.9191080715	-0.8676600476
H	10.6076149336	-1.6708017999	1.2953392355
H	9.7121997389	1.5042504950	-1.4526581999
N	13.2287567123	-1.2733672417	1.1335948179
H	14.1402996520	-0.8527499713	1.1829934154

H	12.9502764682	-1.8173977186	1.9290361505
N	12.2634722760	2.2029572693	-1.7109027359
H	13.2383003648	2.1426425566	-1.9512717549
H	11.6634936729	2.5475249750	-2.4381548654
H	6.4655880899	-3.1578879795	0.0230522882
C	6.7688089847	-2.1179599479	0.0631703736
C	7.5714680340	0.5596323280	0.1406057035
C	5.8300544063	-1.1058974488	0.1796398049
C	8.1111070457	-1.7824777260	-0.0079422005
C	8.5284136824	-0.4511547136	0.0285632501
C	6.2331155374	0.2305857020	0.2190863345
H	8.8527383000	-2.5645446407	-0.1189143733
H	7.8925195110	1.5949280920	0.1853382357
C	4.3667492383	-1.1541498256	0.2832429522
C	1.6349082238	-0.6580098341	0.5352579992
C	3.4771251957	-2.2183018562	0.2863148940
C	3.8936176101	0.1529370046	0.3950853300
C	2.5425047566	0.4028481961	0.5215442898
C	2.1200315831	-1.9615889218	0.4103983715
H	3.8274713155	-3.2409865958	0.2041057684
H	2.1711454209	1.4199097743	0.5915656449
H	1.4202132050	-2.7892068237	0.4389985510
C	5.0320538405	1.1547761732	0.3478948470
C	5.0861518003	1.9813808174	1.6360052824
H	5.9465532711	2.6532590755	1.6317433169
H	5.1607639005	1.3314708572	2.5093733153
H	4.1834988590	2.5879173768	1.7387326842
C	4.8989364374	2.0657677096	-0.8777860309
H	5.7505757800	2.7450720509	-0.9504975563
H	3.9895249855	2.6671527564	-0.8121834090
H	4.8498652132	1.4747372398	-1.7938613639
C	15.5815450411	0.6921870163	-0.9157548109
O	15.3392348883	1.2627465342	-1.8923151039
O	15.8866770289	0.1284313502	0.0463748771
H	-1.9267506794	1.5410629459	2.5359564168
C	-1.6072370212	0.8195761554	1.7927155025
C	-0.7592411458	-1.0573863865	-0.0984081911
C	-2.5295706130	0.1586853682	0.9983402269
C	-0.2604624317	0.5382270126	1.6314664083
C	0.1834048373	-0.3934837544	0.6904208424
C	-2.1028946019	-0.7795491391	0.0554430207
H	0.4665662733	1.0339115634	2.2636994083
H	-0.4243164258	-1.7701694845	-0.8451861772
C	-3.9932327047	0.2454177458	0.9395058918
C	-6.7221251872	-0.0197486721	0.4177479420

C	-4.9036551427	1.0082147577	1.6553050994
C	-4.4437128879	-0.6406677222	-0.0387600975
C	-5.7912190664	-0.7710654838	-0.3028478568
C	-6.2576682958	0.8683652788	1.3903141017
H	-4.5728670454	1.6969999993	2.4239611735
H	-6.1379699886	-1.4450425754	-1.0792260043
H	-6.9752779134	1.4376469546	1.9698335925
C	-3.2867418356	-1.3702718368	-0.6982466828
H	-10.4181066528	-2.6695515403	-0.4827436134
C	-10.0399214226	-1.6686946065	-0.3089037136
C	-9.0467436239	0.9012664194	0.1671638941
C	-10.8903920552	-0.5762356990	-0.3059095069
C	-8.6913647799	-1.4670980120	-0.0703088468
C	-8.1742868642	-0.1908508837	0.1660607327
C	-10.3946326987	0.7057653876	-0.0642347583
H	-8.0248736333	-2.3208580111	-0.0417044074
H	-8.6539723403	1.8993807510	0.3309310795
C	-12.3392652083	-0.4879127126	-0.5180542175
C	-14.9871961044	0.2344651019	-0.8277412106
C	-13.2820345754	-1.4702803584	-0.7832110342
C	-12.7163496670	0.8506306311	-0.4057763384
C	-14.0407260449	1.2168641426	-0.5610056797
C	-14.6100979460	-1.0988042775	-0.9368182159
H	-12.9937704865	-2.5119460369	-0.8682021345
H	-14.3470947892	2.2540444977	-0.4756984917
H	-15.3604127862	-1.8532205152	-1.1423321433
H	-16.0283692553	0.5087291945	-0.9504645305
C	-11.5181605399	1.7320969262	-0.0980915712
C	-3.3991693962	-2.8841009251	-0.4812165095
H	-2.5348703353	-3.4017150723	-0.9027677970
H	-4.2947565981	-3.2744627908	-0.9705132141
H	-3.4603012820	-3.1240576496	0.5812815006
C	-3.2223726721	-1.0558966936	-2.1974086333
H	-2.3548334483	-1.5335543050	-2.6575122722
H	-3.1553310487	0.0192062485	-2.3693269619
H	-4.1171397302	-1.4262116348	-2.7033096717
C	-11.3035305107	2.7737936796	-1.1998886357
H	-11.1939256680	2.2915184594	-2.1724708884
H	-10.4068755188	3.3656093004	-1.0054666258
H	-12.1546734900	3.4563773503	-1.2515955124
C	-11.6869371760	2.4119765494	1.2656749582
H	-12.5432995955	3.0899573953	1.2527981069
H	-10.7987974504	2.9927386911	1.5228258986
H	-11.8521739663	1.6702578473	2.0488965390

TA2-CO_2 in aqueous phase

C	10.0954666242	0.1270983557	0.0991096228
C	11.8786314328	1.5904268741	-0.5354526180
C	12.3994978807	-0.4071599678	0.4637018521
N	12.8070489329	0.7355158223	-0.0981278739
C	11.0526813856	-0.7524563025	0.5889618661
C	10.5081190980	1.3289973185	-0.4600727236
H	10.7738944556	-1.6894726440	1.0535057705
H	9.7976824300	2.0354765430	-0.8699101016
N	13.3857523921	-1.2717506312	0.8677035574
H	14.2966486420	-0.8654795878	1.0035761976
H	13.1311016902	-1.9729102792	1.5428952810
N	12.3422710922	2.7763510598	-1.0501954659
H	13.3029742983	2.7696990082	-1.3520742120
H	11.7187329066	3.2809072280	-1.6581464085
H	6.6246759541	-2.9018562930	-0.4442347993
C	6.9170971527	-1.8924468471	-0.1777441667
C	7.6887067207	0.7191156046	0.4835391128
C	5.9687373894	-0.9407134580	0.1638023439
C	8.2554725579	-1.5302802869	-0.1799424654
C	8.6553587438	-0.2311382584	0.1433037572
C	6.3547262782	0.3598974710	0.4994027100
H	9.0042963979	-2.2622098748	-0.4591987555
H	7.9916734937	1.7269786254	0.7470064921
C	4.5059891737	-1.0289685388	0.2528472547
C	1.7668677122	-0.6283114949	0.5790063248
C	3.6302883254	-2.0774984232	0.0058677879
C	4.0179271945	0.2141080110	0.6567900751
C	2.6619001309	0.4167688207	0.8229726908
C	2.2682460293	-1.8672960508	0.1681405121
H	3.9945253452	-3.0502123954	-0.3056077257
H	2.2839575348	1.3886169397	1.1227387209
H	1.5790861590	-2.6853182538	-0.0099111914
C	5.1440265056	1.2127369773	0.8470739319
C	5.1981404014	1.7055813603	2.2972280560
H	6.0494934957	2.3727752942	2.4446728340
H	5.2906324443	0.8657593214	2.9889647333
H	4.2866495921	2.2544600363	2.5440033858
C	4.9924937043	2.3929424957	-0.1192726981
H	5.8403720265	3.0746598244	-0.0290734020
H	4.0801910792	2.9502491698	0.1043362172
H	4.9365114724	2.0431008612	-1.1521559532
C	12.7767007636	-1.3376939139	-2.7901981260
O	11.6552949788	-1.1491797700	-2.9991368755
O	13.8983422801	-1.5325359193	-2.5899497496

H	-1.8821299694	1.1286295327	2.8577243311
C	-1.5316914377	0.5555888061	2.0065906571
C	-0.6043757977	-0.9385357183	-0.1727863098
C	-2.4222666549	0.0385186468	1.0780039425
C	-0.1749803767	0.3251930550	1.8330511031
C	0.3070127036	-0.4162033481	0.7500275166
C	-1.9562078623	-0.7072071643	-0.0087207606
H	0.5261538545	0.7164547988	2.5609033227
H	-0.2454522104	-1.5032809251	-1.0271828394
C	-3.8861464529	0.1220284705	0.9886619821
C	-6.5937220667	-0.0658157773	0.3327042347
C	-4.8304424579	0.7295910021	1.8049289519
C	-4.2917498235	-0.5691569142	-0.1540054369
C	-5.6283458771	-0.6595379198	-0.4854770469
C	-6.1744945445	0.6290474777	1.4715288170
H	-4.5340552791	1.2667280986	2.6987405206
H	-5.9322891416	-1.1843394795	-1.3849545036
H	-6.9159461133	1.0789449111	2.1218790896
C	-3.1066978791	-1.1574142335	-0.8970003735
H	-10.1887275867	-2.4941356537	-1.3145573812
C	-9.8451576196	-1.5603241683	-0.8838489046
C	-8.9421497616	0.8350162233	0.2513146532
C	-10.7284595430	-0.5227251959	-0.6320539299
C	-8.5083661347	-1.3918745076	-0.5613928209
C	-8.0359343630	-0.2017648806	0.0023651751
C	-10.2786998547	0.6697801428	-0.0614627313
H	-7.8191333136	-2.2100004926	-0.7333925249
H	-8.5913031808	1.7695526453	0.6764608234
C	-12.1752846901	-0.4194309360	-0.8555670726
C	-14.8388479083	0.2901971531	-1.0417261074
C	-13.0802468769	-1.3283870252	-1.3873780936
C	-12.5957434289	0.8379707118	-0.4175110434
C	-13.9290294961	1.1984584011	-0.5088869775
C	-14.4174814275	-0.9629388818	-1.4767056891
H	-12.7555930748	-2.3061825568	-1.7257927167
H	-14.2680279405	2.1717399633	-0.1700130752
H	-15.1398682506	-1.6590696729	-1.8874921428
H	-15.8862011384	0.5594654461	-1.1175805945
C	-11.4320122025	1.6433570513	0.1342326901
C	-3.2077584282	-2.6865138440	-0.9675271030
H	-2.3201665459	-3.1075489535	-1.4441628666
H	-4.0804060532	-2.9798595140	-1.5557374950
H	-3.3055849095	-3.1198758710	0.0296722211
C	-2.9962333201	-0.5745414162	-2.3113253586
H	-2.1073217605	-0.9588238895	-2.8156855667

H	-2.9365094571	0.5151167285	-2.2834449129
H	-3.8702060506	-0.8553274735	-2.9036618939
C	-11.2273599358	2.9363570939	-0.6614630869
H	-11.0843562465	2.7212605685	-1.7223542819
H	-10.3523785551	3.4771517547	-0.2956830483
H	-12.0986748358	3.5866284329	-0.5573095459
C	-11.6487230542	1.9566597652	1.6200827390
H	-12.5241733737	2.5971566059	1.7477582281
H	-10.7816695539	2.4757008354	2.0333152616
H	-11.8086635727	1.0394882813	2.1908194957

TA3 in gas phase

H	9.2469186287	-1.9602438355	-0.3246402409
C	9.9173476396	-1.1419910811	-0.1236168466
C	10.4027897581	1.1807975063	0.2209312228
N	12.1768531763	-0.4269927561	0.1940252111
C	11.7418809069	0.8247289773	0.2911565673
C	11.2765912087	-1.3834837332	0.0007325801
C	9.4725660901	0.1700591787	-0.0003866328
H	10.1151644531	2.2109686208	0.3482628687
N	11.8455598552	-2.6590059734	-0.0784866031
N	12.7803707278	1.7397729267	0.4838147200
H	13.6815044142	1.2952862176	0.5459064666
H	12.8497727651	-2.6427099788	-0.0089379135
C	12.7329488459	3.1096838724	0.5297258275
C	11.2265707937	-3.8810994983	-0.1573037927
O	11.7134098657	3.7540046821	0.4320795915
O	10.0263611628	-4.0293287847	-0.2074618698
C	14.0870742503	3.7518141689	0.7323687603
H	14.8218212171	3.3640834398	0.0246097494
H	14.4475814211	3.5484340236	1.7428547518
H	13.9862648220	4.8255038870	0.6014502599
C	12.1902477479	-5.0466859532	-0.1814609535
H	11.6173265413	-5.9696032168	-0.1894524946
H	12.8430149180	-5.0324187882	0.6934135772
H	12.8173733634	-5.0050326136	-1.0742046331
H	5.9397592359	2.9482597750	-1.1704774425
C	6.2484931717	1.9933814985	-0.7612488837
C	7.0715008956	-0.4711354069	0.2692225044
C	5.3137981430	1.0415949158	-0.3868585468
C	7.5960451849	1.7020276960	-0.6236402391
C	8.0254727465	0.4757251171	-0.1130592986
C	5.7295686139	-0.1893346358	0.1268534513
H	8.3299983051	2.4315324113	-0.9428001617

H	7.3898738304	-1.4224907671	0.6810242453
C	3.8470609473	1.0454930763	-0.4482253890
C	1.1174760000	0.4730241818	-0.4162791352
C	2.9435199401	2.0005109867	-0.8901858890
C	3.3876953335	-0.1853725275	0.0213870702
C	2.0381877783	-0.4714365695	0.0407994225
C	1.5883926782	1.7069643971	-0.8704012786
H	3.2829589545	2.9586181898	-1.2662051950
H	1.6803729706	-1.4246602214	0.4159820568
H	0.8785964488	2.4343190987	-1.2474744387
C	4.5381635969	-1.0819652134	0.4410916598
C	4.5614794108	-2.3664712237	-0.3975756688
H	4.5983326428	-2.1372725655	-1.4636023952
H	3.6647816431	-2.9612760031	-0.2078617580
H	5.4297195098	-2.9793917775	-0.1472064968
C	4.4577730070	-1.4273072540	1.9322473721
H	5.3196810192	-2.0239632811	2.2378504941
H	3.5564836306	-2.0085790876	2.1406925641
H	4.4289162351	-0.5238437317	2.5428138272
H	-2.3963036327	-2.4154243977	-1.3160127907
C	-2.0938326288	-1.4389484007	-0.9554146147
C	-1.2912667094	1.0840483900	-0.0553137803
C	-3.0346108607	-0.5004438368	-0.5653994111
C	-0.7510056618	-1.1061983601	-0.8942021311
C	-0.3301030653	0.1495023268	-0.4495563942
C	-2.6319133533	0.7577693417	-0.1130574453
H	-0.0100086156	-1.8243750848	-1.2250746001
H	-0.9733738686	2.0547476118	0.3107498372
C	-4.4999428746	-0.5592329088	-0.5394432063
C	-7.2430116739	-0.1059613894	-0.3266769222
C	-5.3873406355	-1.5637409729	-0.8952922809
C	-4.9788067699	0.6634056353	-0.0697352374
C	-6.3354443538	0.8901640230	0.0408143489
C	-6.7492527573	-1.3284054107	-0.7878028851
H	-5.0322386702	-2.5177933298	-1.2681268149
H	-6.7084712699	1.8338467532	0.4246394856
H	-7.4486891917	-2.0971068043	-1.0961250245
C	-3.8375761858	1.6078191511	0.2614849109
H	-10.9518918582	2.6210783882	-0.8949314098
C	-10.5769750019	1.6524224199	-0.5847803713
C	-9.5871728015	-0.8472682962	0.1814878826
C	-11.4396145213	0.6585359455	-0.1534658053
C	-9.2187651788	1.3856775064	-0.6335658248
C	-8.7034504369	0.1444686301	-0.2523293461
C	-10.9431614760	-0.5903030850	0.2251759728

H	-8.5410629843	2.1464571468	-1.0017529006
H	-9.1987018149	-1.8101365405	0.4971635013
C	-12.9007407372	0.6419104762	-0.0129245380
C	-15.5705459714	0.0650944693	0.4156126284
C	-13.8535666290	1.6184133557	-0.2627372359
C	-13.2808568565	-0.6192807450	0.4487789502
C	-14.6146520084	-0.9124648532	0.6644639505
C	-15.1914373677	1.3203493987	-0.0448643908
H	-13.5651858932	2.5987305136	-0.6240975420
H	-14.9202911832	-1.8903836588	1.0213725974
H	-15.9486623165	2.0715698741	-0.2356469006
H	-16.6192850128	-0.1527585867	0.5801813697
C	-12.0741710235	-1.5218595737	0.6391855407
C	-3.8380719526	1.9564813010	1.7539133904
H	-3.7998451879	1.0514142740	2.3622611119
H	-4.7446057720	2.5055932791	2.0183053412
H	-2.9781673649	2.5791761846	2.0083697420
C	-3.9155807977	2.8773315068	-0.5924568875
H	-4.8228076698	3.4401180061	-0.3609523716
H	-3.9314108757	2.6278058741	-1.6546404631
H	-3.0583278071	3.5262293937	-0.4027157087
C	-11.9427029331	-1.9688349673	2.0991790465
H	-11.8963159074	-1.1088991576	2.7686388881
H	-11.0400085841	-2.5665702747	2.2419429062
H	-12.7999122296	-2.5808975389	2.3893618006
C	-12.1565075741	-2.7457474380	-0.2821845566
H	-13.0166736808	-3.3657417335	-0.0185757046
H	-11.2588394435	-3.3610714830	-0.1914352454
H	-12.2626330265	-2.4438383791	-1.3252431944

TA3 in aqueous phase

H	9.2690136341	-1.9354958231	-0.2111310322
C	9.9395483502	-1.1083170289	-0.0536377457
C	10.4121656915	1.2322216602	0.1687383341
N	12.1918985245	-0.3651103841	0.2390762652
C	11.7544133996	0.8899234852	0.2690865995
C	11.3005055697	-1.3389655508	0.0894313216
C	9.4878003347	0.2064183996	-0.0037108780
H	10.1130619900	2.2643605081	0.2349095856
N	11.8787465285	-2.6119860725	0.0797582528
N	12.7878716704	1.8170718456	0.4235007279
H	13.6958884435	1.3895377897	0.5196755880
H	12.8842872943	-2.5964187336	0.1506849451
C	12.7354283608	3.1798253369	0.4194592895
C	11.2744789631	-3.8347039035	0.0421689444

O	11.7028774897	3.8153418331	0.2827099182
O	10.0655366955	-3.9894783362	-0.0180666613
C	14.0638893713	3.8606801411	0.6183473603
H	14.9118489593	3.1876151301	0.5055031433
H	14.0812986711	4.2857205970	1.6236643595
H	14.1459790865	4.6796312887	-0.0948735792
C	12.2160838457	-5.0100960476	0.0667945402
H	11.8788870744	-5.7053623326	0.8351914638
H	13.2513698790	-4.7323438511	0.2547575281
H	12.1510158084	-5.5188403234	-0.8963430891
H	5.9474408766	2.9090652248	-1.3347918191
C	6.2590728601	1.9786297251	-0.8741230644
C	7.0861559700	-0.4293805851	0.2904105796
C	5.3265030257	1.0444428862	-0.4494399850
C	7.6079990961	1.6968654055	-0.7179892872
C	8.0387136121	0.4998262897	-0.1398604516
C	5.7431676733	-0.1580643693	0.1291902363
H	8.3392079351	2.4116964100	-1.0750512105
H	7.4006593675	-1.3578151879	0.7542674599
C	3.8590994452	1.0428298558	-0.5118122365
C	1.1298989089	0.4681746487	-0.4469963453
C	2.9541603373	1.9745736511	-1.0020804133
C	3.4025588073	-0.1637825160	0.0208420030
C	2.0530406949	-0.4518023050	0.0570114600
C	1.5983331265	1.6797925672	-0.9648702279
H	3.2928058497	2.9134630317	-1.4250590472
H	1.7039041393	-1.3885143802	0.4785993933
H	0.8889297537	2.3914866637	-1.3717198251
C	4.5535553989	-1.0373073221	0.4837608699
C	4.5807279906	-2.3592003432	-0.2954177630
H	4.6226148443	-2.1797248621	-1.3715037669
H	3.6822721916	-2.9420901553	-0.0798980099
H	5.4490484111	-2.9561771955	-0.0090871402
C	4.4714427861	-1.3169048425	1.9885643951
H	5.3362461025	-1.8968816679	2.3171310801
H	3.5712489518	-1.8925131353	2.2158334634
H	4.4382229912	-0.3873303361	2.5596869253
H	-2.3731363181	-2.5191086277	-1.0298877386
C	-2.0750066811	-1.5063037826	-0.7831376251
C	-1.2849286068	1.1102461133	-0.1703721359
C	-3.0198638698	-0.5334763249	-0.4967021857
C	-0.7330299660	-1.1609620654	-0.7600587652
C	-0.3186562410	0.1398629799	-0.4557764753
C	-2.6245806193	0.7711457942	-0.1898378090
H	0.0091793661	-1.9125387051	-1.0021750410

H	-0.9786516096	2.1200154024	0.0822315372
C	-4.4850012221	-0.5998268667	-0.4509623831
C	-7.2302603529	-0.1446188041	-0.2578052073
C	-5.3672359616	-1.6460083382	-0.6830924030
C	-4.9687156453	0.6645499060	-0.1137167961
C	-6.3266333518	0.8938840612	-0.0130332136
C	-6.7309890577	-1.4090353937	-0.5862979376
H	-5.0075234781	-2.6334763950	-0.9502274354
H	-6.6964682770	1.8752420595	0.2642640882
H	-7.4242003038	-2.2164579623	-0.7933901179
C	-3.8337995388	1.6502488987	0.0948259268
H	-10.9537143541	2.5327185147	-0.9811399599
C	-10.5743520271	1.5838359004	-0.6187436400
C	-9.5744924174	-0.8696570134	0.2873675802
C	-11.4332544499	0.6079986608	-0.1377861856
C	-9.2135793558	1.3212389214	-0.6472289040
C	-8.6937202103	0.1031055804	-0.1975068773
C	-10.9327792431	-0.6165706473	0.3112934666
H	-8.5407477742	2.0694139437	-1.0487561171
H	-9.1889291482	-1.8163060601	0.6516315169
C	-12.8959470801	0.5897739310	-0.0073934681
C	-15.5661494804	0.0183968217	0.4284106802
C	-13.8517195590	1.5473710501	-0.3192404833
C	-13.2713689204	-0.6485040915	0.5185751044
C	-14.6062596689	-0.9395975449	0.7390359690
C	-15.1908883832	1.2513154114	-0.0968323304
H	-13.5642524952	2.5082914779	-0.7309276269
H	-14.9072181664	-1.8995650910	1.1455158523
H	-15.9515823401	1.9857866685	-0.3351325680
H	-16.6153851156	-0.1973086715	0.5952462552
C	-12.0609454444	-1.5317269271	0.7670227037
C	-3.8236333271	2.1724569734	1.5358331073
H	-3.7679322799	1.3460854991	2.2474240583
H	-4.7349941226	2.7392312751	1.7388519853
H	-2.9681765756	2.8305340414	1.6998285009
C	-3.9340101022	2.8123289080	-0.8991886785
H	-4.8460167559	3.3857471715	-0.7191058420
H	-3.9587223508	2.4427644637	-1.9264304533
H	-3.0806318347	3.4847357136	-0.7925281860
C	-11.9387848745	-1.9003225180	2.2498239640
H	-11.9018027392	-1.0059057600	2.8745074622
H	-11.0337978227	-2.4854625554	2.4258025773
H	-12.7967113856	-2.5010131565	2.5604954455
C	-12.1275682731	-2.8051818830	-0.0865765970
H	-12.9869885510	-3.4126520913	0.2065394714

H	-11.2254984289	-3.4051959351	0.0497074772
H	-12.2256183690	-2.5623819977	-1.1465358579

TA3-CO_2 in gas phase

H	9.0250789067	-2.3370813621	-0.3291984337
C	9.4503253714	-1.3549184910	-0.2043287829
C	9.2745671809	0.9948823643	0.2560075822
C	10.6388429786	1.0812485950	0.0169400969
C	10.8041981360	-1.1520131649	-0.4250051624
C	8.6764435336	-0.2547802376	0.1439823692
H	8.7193208143	1.8719444084	0.5457475678
N	11.6836372720	-2.1717727462	-0.7969474557
N	11.3674734011	2.2680444440	0.1162462017
H	12.3513910814	2.1432406077	-0.0545405124
H	12.6264040813	-1.8521553998	-0.9439181595
C	10.9242347488	3.5361667197	0.3897796064
C	11.4367816227	-3.5107744177	-0.9633600456
O	9.7671623324	3.8189681922	0.6055602330
O	10.3525575356	-4.0265902696	-0.8098857305
C	12.0140727382	4.5834669199	0.3731391923
H	13.0127222852	4.1682152701	0.5081381671
H	11.8078642245	5.3101542779	1.1560312428
H	11.9788497602	5.1031994021	-0.5860132147
C	12.6576952610	-4.3211988362	-1.3354972667
H	12.3629057035	-5.0719857650	-2.0658629184
H	13.0104799000	-4.8422457375	-0.4437539338
H	13.4735159427	-3.7185779572	-1.7342489048
H	5.0777628215	-2.5547209154	1.9454386944
C	5.4147338319	-1.7025592735	1.3667709360
C	6.3068508215	0.5007496926	-0.1099241488
C	4.5120648496	-0.7835084114	0.8569622340
C	6.7657199786	-1.5204574418	1.1221317471
C	7.2250128124	-0.4233879202	0.3922882547
C	4.9581122227	0.3110598341	0.1125768136
H	7.4814676913	-2.2320257229	1.5159955199
H	6.6603254364	1.3440995063	-0.6936351822
C	3.0478056018	-0.7275348287	0.9331986978
C	0.3294170379	-0.1370705862	0.7469980049
C	2.1244467270	-1.5670611222	1.5380119238
C	2.6160811452	0.3979384780	0.2318010920
C	1.2713900694	0.6937859874	0.1371579709
C	0.7751450037	-1.2648259195	1.4404276064
H	2.4423817953	-2.4456624955	2.0876436551
H	0.9338659825	1.5554247568	-0.4293338654

H	0.0489871632	-1.9023539529	1.9315896865
C	3.7860664889	1.1468052558	-0.3793099522
C	3.8537082477	2.5879693224	0.1324067428
H	3.9020306426	2.6110194430	1.2220181591
H	2.9693179266	3.1468248514	-0.1821128880
H	4.7334403265	3.0999576352	-0.2621951943
C	3.6947024292	1.1210986064	-1.9107938864
H	4.5693794285	1.5949895005	-2.3605353555
H	2.8061249614	1.6586131593	-2.2495917935
H	3.6316061284	0.0955268769	-2.2784646012
N	11.3941567690	0.0361995567	-0.3169641826
C	14.4450844430	0.3206451539	-0.7975920813
O	14.3978255502	1.4426550053	-0.5233856302
O	14.5348040663	-0.7973806877	-1.0788639910
H	-3.2181553771	2.8540127056	0.8726829707
C	-2.9030214014	1.8243145021	0.7483633207
C	-2.0638314161	-0.8262240775	0.4599145378
C	-3.8297656493	0.8140406706	0.5496083081
C	-1.5573080630	1.4988197121	0.8062612437
C	-1.1174602214	0.1806104466	0.6666202232
C	-3.4058383050	-0.5092508003	0.4043627237
H	-0.8295237347	2.2795216386	0.9921441829
H	-1.7341581881	-1.8516693972	0.3274554178
C	-5.2954075366	0.8433447847	0.4701893259
C	-8.0272656960	0.2981036657	0.3159015469
C	-6.2070388489	1.8839638694	0.5678835838
C	-5.7472537400	-0.4627310089	0.2796462777
C	-7.0968667438	-0.7363805445	0.2017431815
C	-7.5633373026	1.6034197381	0.4891679107
H	-5.8754316499	2.9042174742	0.7217956110
H	-7.4475649970	-1.7508552723	0.0417910408
H	-8.2828759468	2.4068983561	0.5978523418
C	-4.5902596582	-1.4417799328	0.1929653282
H	-11.6904986763	-2.2572103684	1.5562191854
C	-11.3265737145	-1.4087852399	0.9881054451
C	-10.3673362894	0.7874965139	-0.4535129572
C	-12.1929895092	-0.6197778713	0.2502717172
C	-9.9780963451	-1.0941748671	0.9962917574
C	-9.4798314251	-0.0019130638	0.2821664367
C	-11.7130164410	0.4756762537	-0.4694600523
H	-9.2950928280	-1.6940617001	1.5861578659
H	-9.9864888530	1.6249446506	-1.0290477021
C	-13.6428516375	-0.7162526473	0.0448181632
C	-16.2956015513	-0.4426794788	-0.6773308963
C	-14.5735440317	-1.6225531083	0.5310501432

C	-14.0345076523	0.3220089444	-0.8014021092
C	-15.3611309543	0.4633318139	-1.1649465276
C	-15.9037771995	-1.4780012583	0.1629067463
H	-14.2738128651	-2.4336474686	1.1847805084
H	-15.6772385428	1.2660160049	-1.8227311266
H	-16.6441062037	-2.1778103842	0.5323052110
H	-17.3381577000	-0.3435712404	-0.9560458033
C	-12.8443327596	1.1704183094	-1.2145061719
C	-4.6867026808	-2.5070306829	1.2909944366
H	-5.5803664009	-3.1197419206	1.1500812879
H	-4.7413217849	-2.0485098025	2.2793861163
H	-3.8199380300	-3.1709761540	1.2659967813
C	-4.5424988351	-2.1114120400	-1.1862685692
H	-5.4393137626	-2.7138716902	-1.3491275871
H	-3.6752916611	-2.7701736021	-1.2671517840
H	-4.4844491651	-1.3666868462	-1.9811794444
C	-13.0169464608	2.6217124294	-0.7550807003
H	-13.1795149540	2.6710510461	0.3226187569
H	-13.8755094971	3.0807568351	-1.2506210155
H	-12.1321007111	3.2135006096	-0.9984489277
C	-12.6362931703	1.1085739627	-2.7323572704
H	-12.5276710740	0.0759947166	-3.0679795460
H	-11.7415540428	1.6616169607	-3.0253122847
H	-13.4900835369	1.5474214886	-3.2538169326

TA3-CO_2 in aqueous phase

H	9.0776331753	-2.2286440118	-0.6385073331
C	9.5016491354	-1.2751340577	-0.3727910179
C	9.3046843887	0.9865077727	0.4067391093
C	10.6779621889	1.1037936035	0.2300389468
C	10.8621386123	-1.0455727916	-0.5255653745
C	8.7139566133	-0.2347545614	0.1044918525
H	8.7316915338	1.8113042966	0.7959353674
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C	12.0596804109	4.4819988346	1.1800091263
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